

Cyanobiphenyl versus Alkoxybiphenyl: Which Mesogenic Unit Governs the Mesomorphic Properties of Guanidinium Ionic Liquid Crystals?

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Supplementary Material

Syntheses

N-{3-[(10-Bromodecyl)oxy]phenyl}acetamide (*m*-5) analogous to Ref.^[70]

1,10-Dibromodecane (2.7 mL, 3.59 g; 11.9 mmol) was added to a solution of *N*-(3-hydroxyphenyl)acetamide **4** (301 mg, 1.99 mmol) and K₂CO₃ (881 mg, 6.37 mmol) in MeCN (30 mL), and the reaction mixture heated for 17 h at 100 °C. Silica (ca. 500 mg) was added to the mixture and the solvent removed under reduced pressure. The residue was purified by chromatography (silica; 5 : 1 hexanes/EtOAc to remove excess bromodecane, then 3 : 1 → 1 : 1 hexanes/EtOAc) to give *m*-**5** (1.05 g, 5.11 mmol, 58 %) as a colorless solid, mp 65 °C. $\nu_{\max}/\text{cm}^{-1}$ 3303 (w), 2938 (m), 2918 (m), 2853 (m), 1663 (s), 1611 (m), 1592 (s), 1490 (m), 1474 (m), 1448 (m), 1431 (s), 1393 (m), 1363 (m), 1334 (w), 1296 (m), 1274 (s), 1246 (m), 1215 (w), 1177 (s), 1151 (m), 1083 (w), 1039 (m), 1013 (m), 996 (w), 984 (w), 968 (w), 955 (w), 871 (w), 845 (w), 832 (w), 783 (m), 767 (m), 717 (s), 681 (s), 662 (w), 641 (m), 617 (m), 595 (w), 582 (w), 531 (m). δ_{H} (500 MHz, CDCl₃) 1.26–1.48 (m, 12H, 6 × CH₂), 1.72–1.80 (m, 2H, BrCH₂CH₂), 1.82–1.88 (m, 2H, OCH₂CH₂), 2.17 (s, 3H, CH₃), 3.41 (t, *J* 6.9, 2H, BrCH₂), 3.94 (t, *J* 6.6, 2H, OCH₂), 6.65 (m, 1H, 4-H), 6.92 (m, 1H, 6-H), 7.19 (m, 2H, 5-H, NH), 7.27 (m, 1H, 2-H). δ_{C} (126 MHz, CDCl₃): δ = 24.7, 26.0, 28.2, 28.7, 29.2, 29.3, 29.4, 32.8, 34.1 (CH₃, 9 × CH₂), 68.0 (OCH₂), 106.2, 110.7, 111.7 (C-2, C-4, C-6), 129.6 (C-5), 139.0 (C-1), 159.7 (C-3), 168.2 (C=O). *m/z* (EI) (%) 369 (78) [M⁺], 151 (42), 109 (100). Anal. Calc. for C₁₈H₂₈BrNO₂: C 58.38, H 7.62, N 3.78, Br 21.58. Found: C 58.48, H 7.60, N 3.71, Br 21.36.

General Procedure for the Williamson Etherification with Biphenyl-4-ols 6 analogous to Ref.^[71]

Biphenyl-4-ol **6a** or **6b** (1.54 mmol), the respective bromide **5** (1.40 mmol) and K₂CO₃ (4.90 mmol) were suspended in MeCN (40 mL) and the reaction mixture heated at 85 °C (for **7a**) or 110 °C (for **7b**) for the given time. In the case of **7a**, H₂O (15 mL) was added, the solid filtered off, washed with H₂O (20 mL) and MeCN (40–80 mL) and recrystallized. Workup of **7b** is given for the respective product.

N-{4-[(10-[[4'-(Decyloxy)-1,1'-biphenyl-4-yl]oxy]decyl)oxy]phenyl}acetamide (*p*-**7a**). Reaction time 17 h, recrystallization from THF afforded *p*-**7a** (695 mg, 1.13 mmol, 81 %) as a colorless solid, mp 181 °C. $\nu_{\max}/\text{cm}^{-1}$ 3286 (w), 3256 (w), 3195 (w), 3136 (w), 3069 (w), 3042 (w), 2957 (w), 2937 (m), 2919 (m), 2876 (w), 2849 (m), 1659 (m), 1606 (m), 1552 (m), 1530 (w), 1499 (m), 1474 (m), 1462 (m), 1410 (w), 1393 (w), 1372 (w), 1328 (w), 1302 (w), 1274 (m), 1248 (s), 1231 (w), 1177 (m), 1166 (w), 1139 (w), 1107 (w), 1082 (w), 1048 (w), 1032 (m), 1011 (m), 995 (w), 978 (w), 953 (w), 932 (w), 914 (w), 890 (w), 869 (w), 824 (s), 809 (m), 797 (m), 765 (w), 745 (w), 718 (w), 671 (w), 644 (w), 594 (m), 550 (w). δ_{H} 0.86 (t, *J* 7.0, 3H, CH₂CH₃), 1.22–1.47 (m, 26H, 13 × CH₂), 1.65–1.75 (m, 6H, 3 × OCH₂CH₂), 1.98 (s, 3H, COCH₃), 3.92 (t, *J* 6.5, 2H, OCH₂), 3.97–4.0 (m, 4H, 2 × OCH₂), 6.78–6.83 (m, 2H, 3-H), 6.92–6.98 (m, 4.9 Hz, 4H, 3'-H, 3''-H), 7.37–7.42 (m, 2H, 2-H), 7.44–7.48 (m, 4H, 2'-H, 2''-H), 9.29 (s, 1H, NH).: *m/z* (ESI) 638 [M+Na⁺], 616 [M+H⁺]. HRMS *m/z* (ESI) calc. for C₄₀H₅₇NNaO₄⁺ 638.4180 [M+Na⁺]. Found: 638.4167. Anal. Calc. for C₄₀H₅₇NO₄: C 78.01, H 9.33, N 2.27. Found: C 77.79, H 9.30, N 2.28.

N-{4-[(10-[[4'-(Cyano)-1,1'-biphenyl-4-yl]oxy]decyl)oxy]phenyl}acetamide (*p*-**7b**). Reaction time 2.5 d, the suspension was filtered, the solid heated in H₂O (50 mL), filtered off and washed with hot H₂O (20 mL) and cold MeOH (5 mL), affording *p*-**7b** (430 mg, 887 μmol, 59 %) as a colorless solid, mp 186 °C. $\nu_{\max}/\text{cm}^{-1}$ 3277 (w), 3251 (w), 3189 (w), 3129 (w), 3073 (w), 3043 (w), 2936 (m), 2920 (m), 2851 (w), 2228 (w), 1655 (m), 1602 (m), 1580 (w), 1543 (w), 1525 (m), 1509 (m), 1493 (m), 1473 (m), 1461 (m), 1409 (w), 1393 (w), 1373 (m), 1320 (w), 1287 (w), 1267 (m), 1250 (s), 1228 (m), 1212 (m), 1181 (m), 1167 (m), 1136 (w), 1115 (w), 1102 (w), 1083 (w), 1046 (m), 1021 (m), 1016 (m), 999 (m), 980 (w), 959 (w), 914 (w), 857 (w), 818 (s), 797 (m), 775 (w), 763 (w), 745 (w), 731 (w), 717 (w), 661 (w), 642 (w), 605 (w), 594 (w), 564 (w). δ_{H} 1.26–1.47 (m, 12H, 6 × CH₂), 1.64–1.77 (m, 4H, 2 × OCH₂CH₂), 1.98 (s, 3H, CH₃), 3.89–4.05 (m, 4H, 2 × OCH₂), 6.79–6.84 (m, 2H, 3-H),

7.01–7.05 (m, 2H, 3'-H), 7.39–7.45 (m, 2H, 2-H), 7.62–7.67 (m, 2H, 2'-H), 7.77–7.83 (m, 4H, 2''-H, 3''-H), 9.42–9.50 (m, 1H, NH). m/z (ESI) 507 $[M+Na^+]$, 397, 371, 327. HRMS m/z (ESI) calc. for $C_{31}H_{36}N_2NaO_3^+$ 507.2618 $[M+Na^+]$. Found: 507.2607. Anal. Calc. for $C_{31}H_{36}N_2O_3$: C 76.83, H 7.49, N 5.78. Found: C 77.11, H 7.57, N 5.59.

N-{3-[(10-[[4'-(Decyloxy)-1,1'-biphenyl-4-yl]oxy]decyl)oxy]phenyl}acetamide (***m*-7a**). Reaction time 17 h, recrystallization from EtOAc afforded ***m*-7a** (719 mg, 1.17 mmol, 83 %) as a colorless solid, mp 140 °C. ν_{max}/cm^{-1} 3299 (w), 3203 (w), 3140 (w), 3068 (w), 3040 (w), 2958 (w), 2937 (m), 2920 (m), 2873 (w), 2852 (m), 1664 (w), 1601 (m), 1568 (w), 1543 (w), 1496 (s), 1474 (m), 1461 (m), 1425 (m), 1393 (w), 1368 (w), 1328 (w), 1300 (w), 1289 (s), 1245 (s), 1178 (m), 1153 (w), 1137 (w), 1082 (w), 1045 (m), 1031 (m), 1010 (m), 994 (w), 980 (w), 952 (w), 925 (w), 823 (s), 807 (m), 768 (w), 742 (w), 718 (w), 685 (w), 665 (w), 646 (w), 616 (w), 594 (m), 540 (w). δ_H 0.86 (t, J 7.0, 3H, CH_2CH_3), 1.22–1.49 (m, 26H, $13 \times CH_2$), 1.64–1.77 (m, 6H, $3 \times OCH_2CH_2$), 2.01 (s, 3H, $COCH_3$), 3.92 (t, J 6.5, 2H, C3- OCH_2), 3.99 (t, J 6.5, 4H, $2 \times$ biphenyl- OCH_2), 6.54–6.61 (m, 1H, 4-H), 6.93–6.98 (m, 4H, 3'-H, 3''-H), 7.02–7.08 (m, 1H, 6-H), 7.08–7.15 (m, 1H, 5-H), 7.21–7.25 (m, 1H, 2-H), 7.41–7.51 (m, 4H, 2'-H, 2''-H), 9.49 (s, 1H, NH). δ_C 13.1 (CH_2CH_3), 21.4, 24.9, 28.0, 28.1, 28.2, 28.3, 30.6 ($16 \times CH_2$, $COCH_3$), 67.3, 67.5 ($3 \times OCH_2$), 105.8, 109.0, 111.3 (C-2, C-4, C-6), 114.7 (C-3', C-3''), 126.6 (C-2', C-2''), 128.6 (C-5), 132.1 (C-1', C-1''), 148.8 (C-1), 157.5 (C-3), 158.6 (C-4', C-4''), 167.6 (C=O). m/z (ESI) 638 $[M+Na^+]$. HRMS m/z (ESI) calc. for $C_{40}H_{57}NNaO_4^+$ 638.4180 $[M+Na^+]$. Found: 638.4159. Anal. Calc. for $C_{40}H_{57}NO_4$: C 78.01, H 9.33, N 2.27. Found: C 77.76, H 9.24, N 2.20.

N-{3-[(10-[[4'-(Cyano)-1,1'-biphenyl-4-yl]oxy]decyl)oxy]phenyl}acetamide (***m*-7b**). Reaction time 53 h; after removal of solvent, CH_2Cl_2 (20 mL) and H_2O (15 mL) were added, the phases separated and the aqueous layer extracted with CH_2Cl_2 (3×5 mL); the combined organic layers were dried ($MgSO_4$), silica was added and the solvent removed under reduced pressure; purification by chromatography (silica; 5 : 1 → 1 : 1 hexanes/EtOAc) afforded ***m*-7b** (331 mg, 683 μ mol, 87 %) as a colorless solid, mp 128 °C. ν_{max}/cm^{-1} 3341 (w), 3316 (w), 2936 (w), 2920 (w), 2851 (w), 2221 (w), 1665 (m), 1597 (s), 1544 (m), 1493 (m), 1470 (m), 1435 (m), 1389 (w), 1365 (w), 1338 (w), 1290 (m), 1252 (s), 1215 (w), 1178 (m), 1157 (s), 1051 (m), 1027 (m), 1010 (m), 997 (w), 955 (w), 932 (w), 865 (m), 850 (w), 820 (m), 766 (m), 729 (m), 709 (m), 685 (m), 662 (w), 608 (w), 583 (w), 561 (w). δ_H 1.29–1.51 (m, 12H, $6 \times CH_2$), 1.72–1.85 (m, 4H, $2 \times OCH_2CH_2$), 2.16 (s, 3H, CH_3), 4.00 (t, J 6.5, 4H, $2 \times OCH_2$), 6.63–6.94 (m, 2H, 4-H, 6-H), 6.97–7.01 (m, 2H, 3'-H), 7.16–7.21 (m, 1H, 5-H), 7.24 (s, 1H, NH), 7.28–

7.31 (m, 1H, 2-H), 7.49–7.54 (m, 2H, 2'-H), 7.64 (m, 2H, 2''-H), 7.66–7.70 (m, 2H, 3''-H). δ_C 24.7, 26.0, 29.2, 29.3, 29.5 (CH₃, 8 × CH₂), 68.0, 68.2 (2 × OCH₂), 106.1 (C-2), 110.0, 110.6, 111.6 (C-4, C-6, C-4''), 115.1 (C-3'), 119.2 (CN), 127.1 (C-2''), 128.3 (C-2'), 129.6 (C-5), 131.2 (C-1'), 132.6 (C-3''), 139.1 (C-1), 145.3 (C-1''), 159.7, 159.8 (C-3, C-4'), 168.3 (C=O). m/z (ESI) 507 [M+Na⁺], 485 [M+H⁺], 393. HRMS m/z (ESI) calc. for C₃₁H₃₆N₂NaO₃⁺ 507.2618 [M+Na⁺]. Found: 507.2608. Anal. Calc. for C₃₁H₃₆N₂O₃: C 76.83, H 7.49, N 5.78. Found: C 76.62, H 7.45, N 5.63.

Hydrolysis of Acetamide

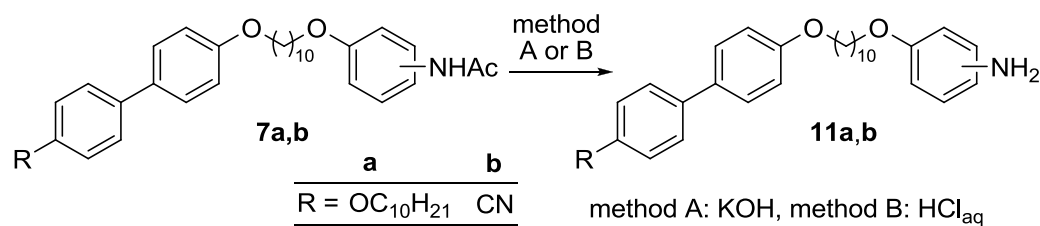


Table S1. Attempted hydrolysis of acetamides 7 under various conditions

Compd	Method	Solvent	T [°C]	t [h]	Product	Remarks
<i>p</i> -7a	B	EtOH	100	64	<i>p</i> -11a	– (no conversion)
<i>p</i> -7a	B	toluene	130	47	<i>p</i> -11a	– (no conversion)
<i>m</i> -7a	B	1,4-dioxane	110	41	<i>m</i> -11a	– (no conversion)
<i>m</i> -7a	B	EtOH	100	64	<i>m</i> -11a	94%
<i>p</i> -7b	A	EtOH	r.t.→100	72	<i>p</i> -11b	– (decomposition)
<i>p</i> -7b	B	EtOH	100	23	<i>p</i> -11b	– (impossible purification)
<i>m</i> -7b	A	EtOH	100	24	<i>m</i> -11b	– (decomposition)
<i>m</i> -7b	B	EtOH	100	27	<i>m</i> -11b	– (impossible purification)

Effect of concentrations on the N–H signal of *m*-**3b** · Cl

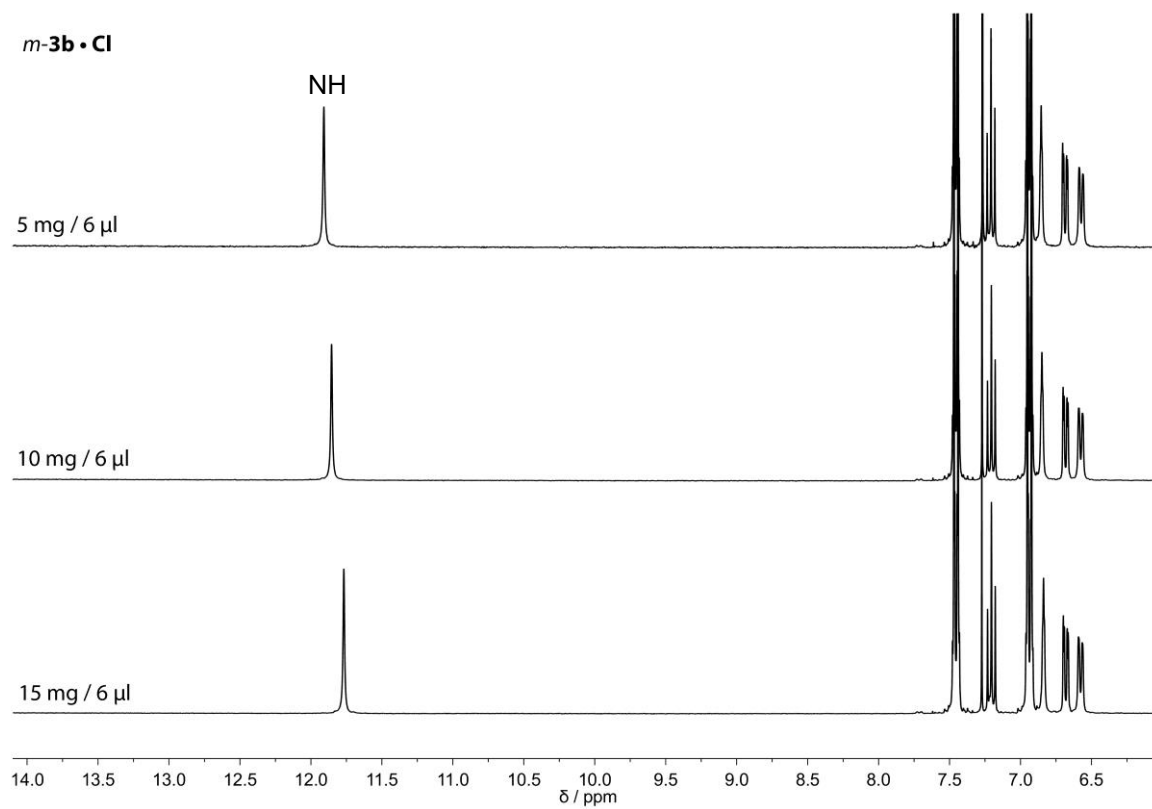
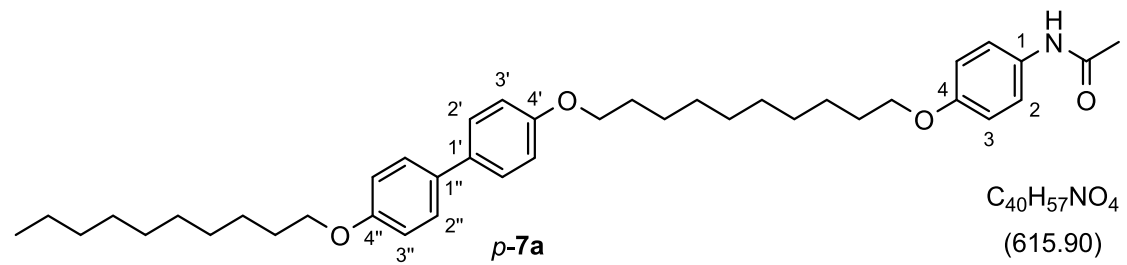
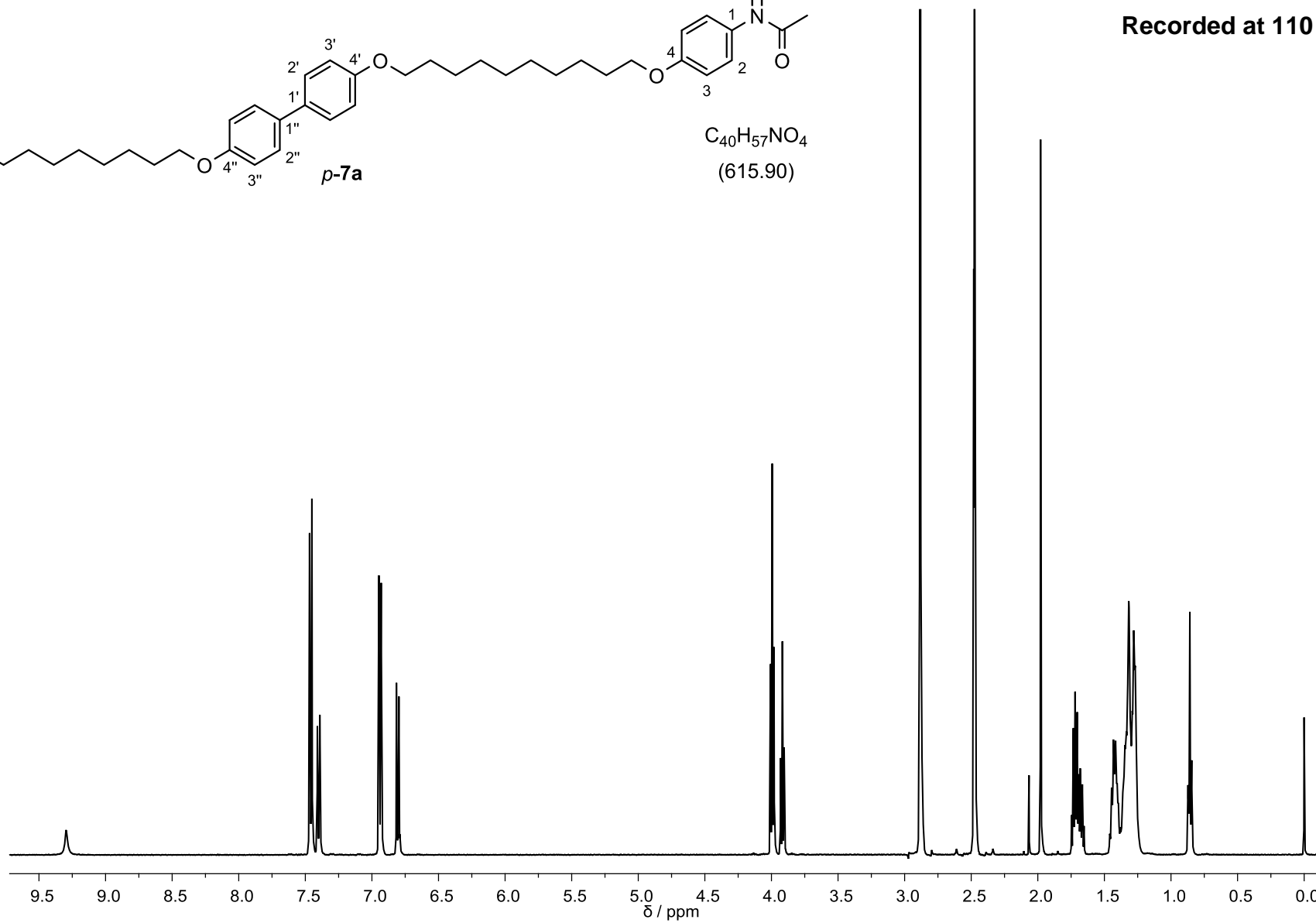


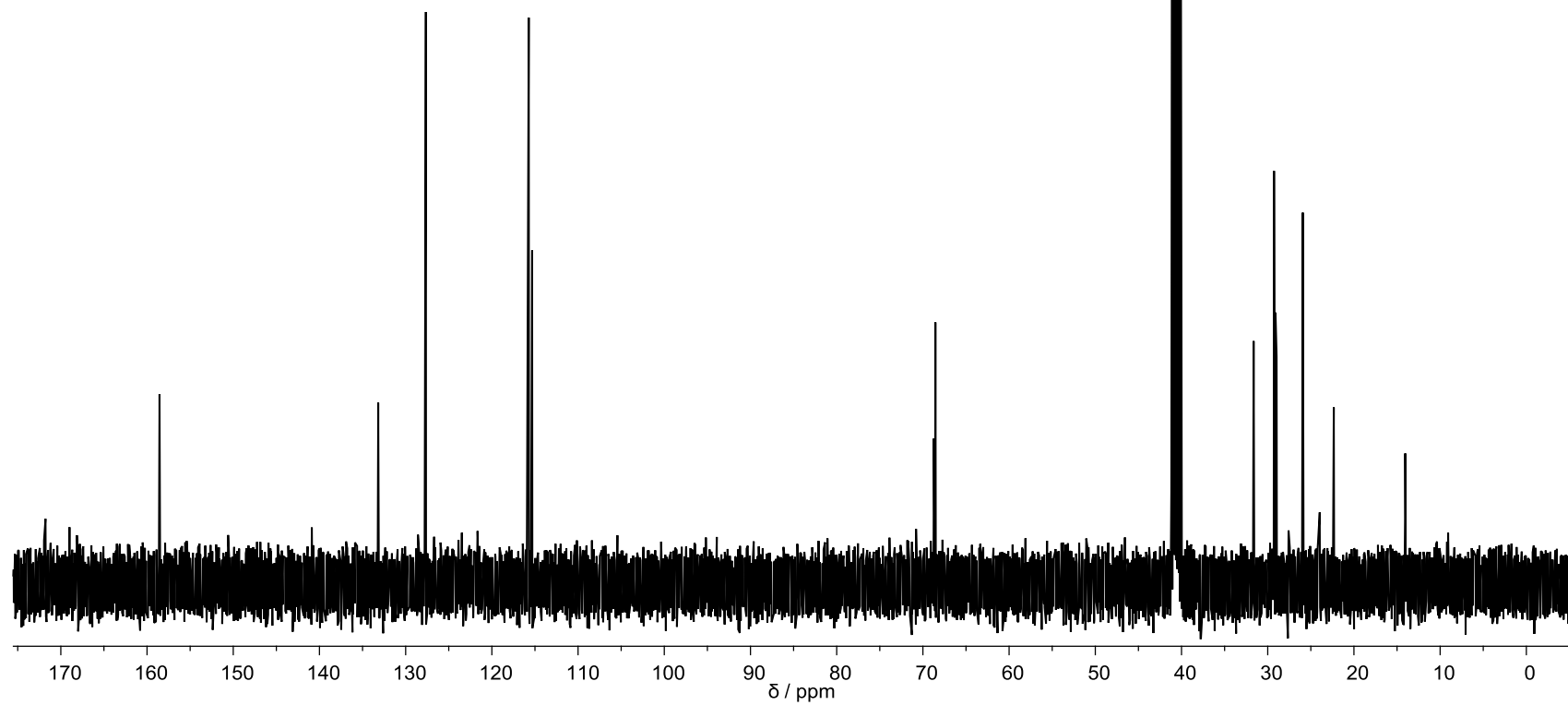
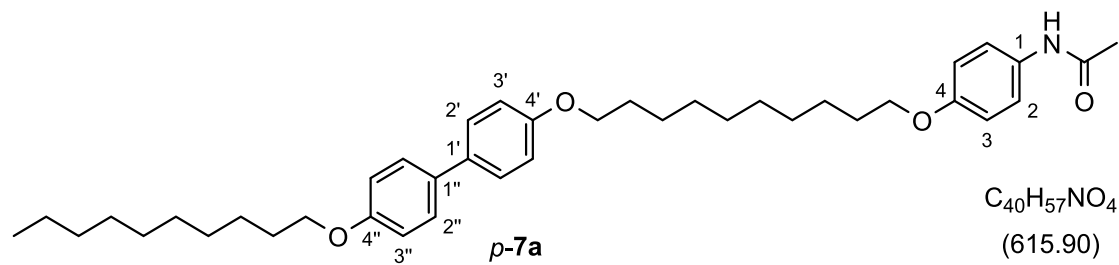
Fig. S1. ¹H NMR spectra of *m*-**3b** · Cl at various concentrations in CDCl₃.



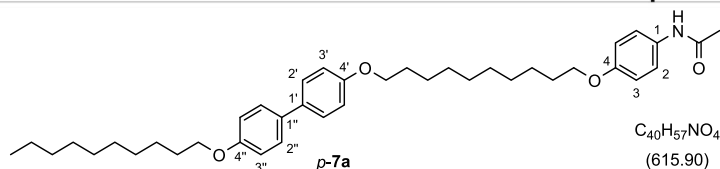
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Recorded at 110 °C



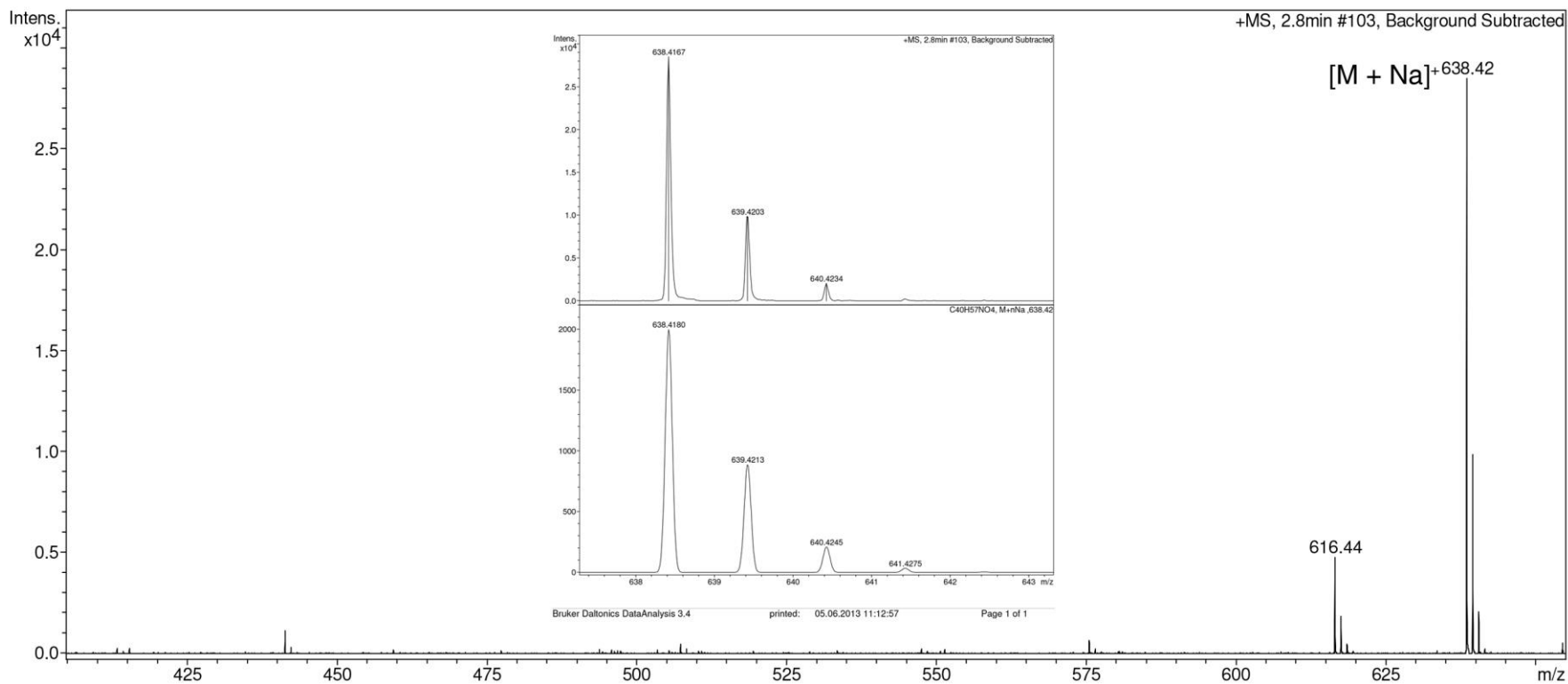
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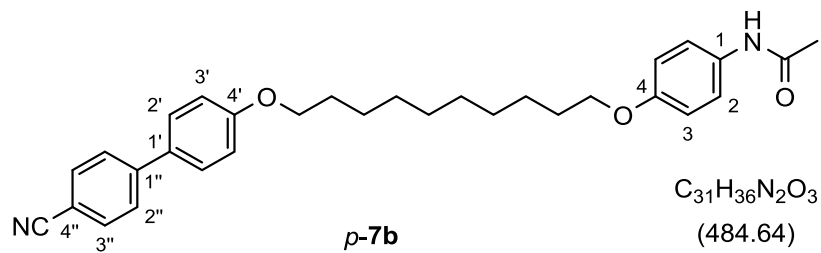


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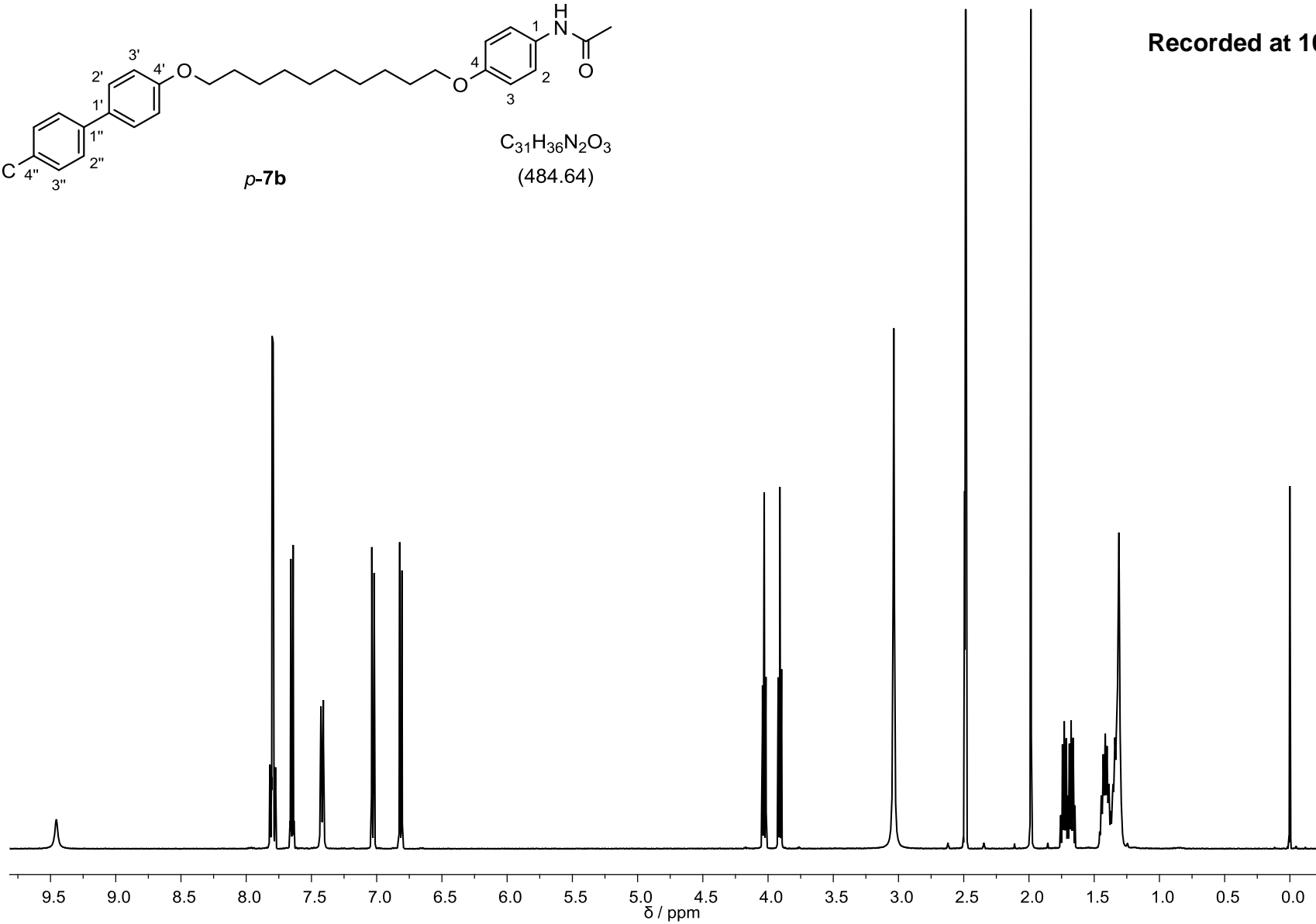
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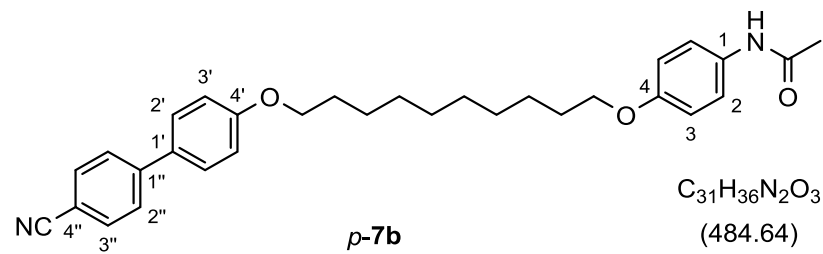
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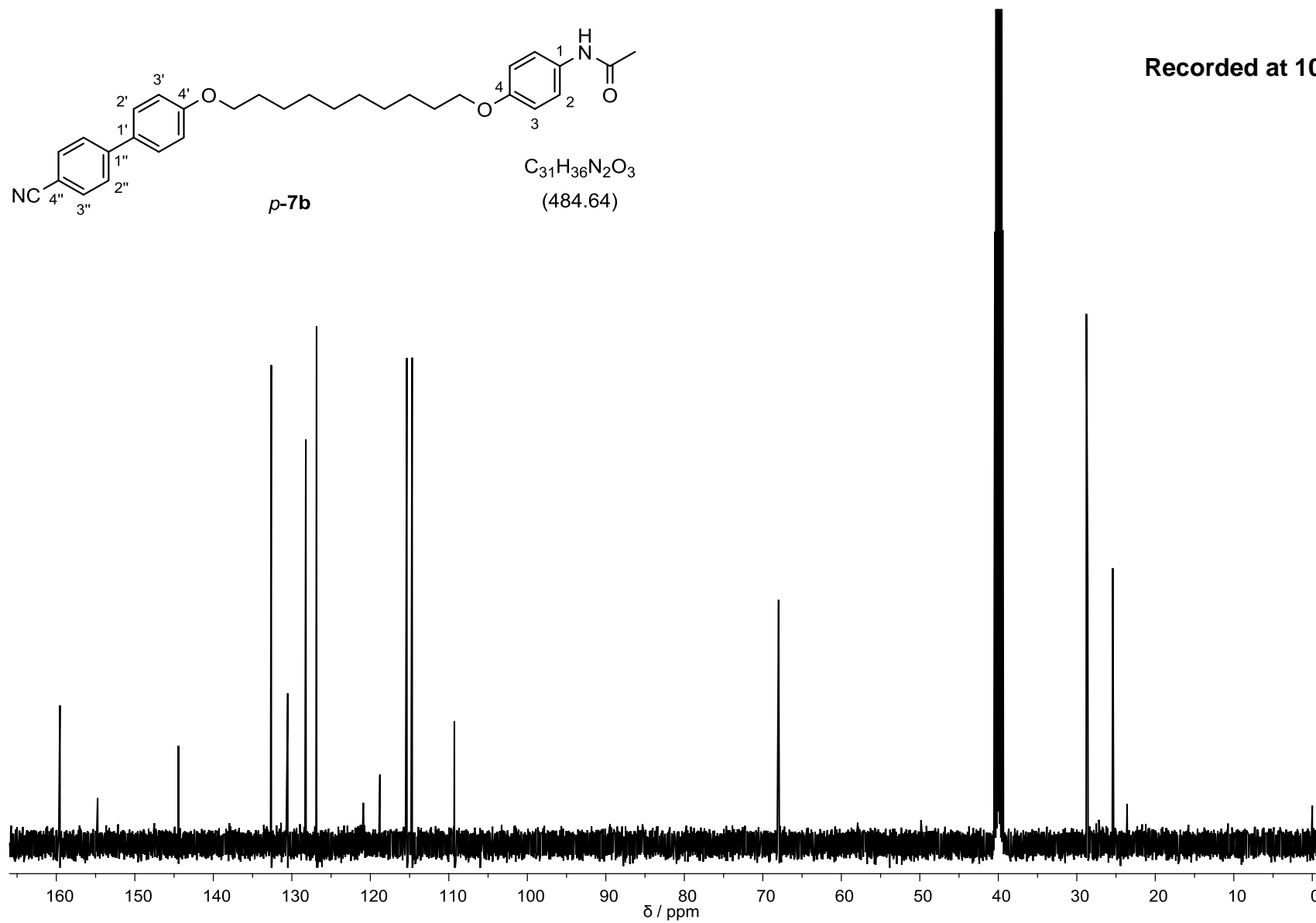


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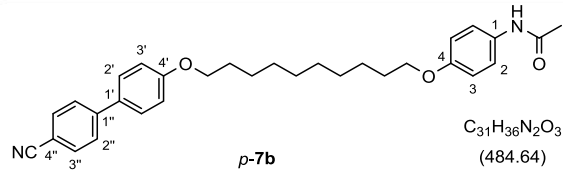




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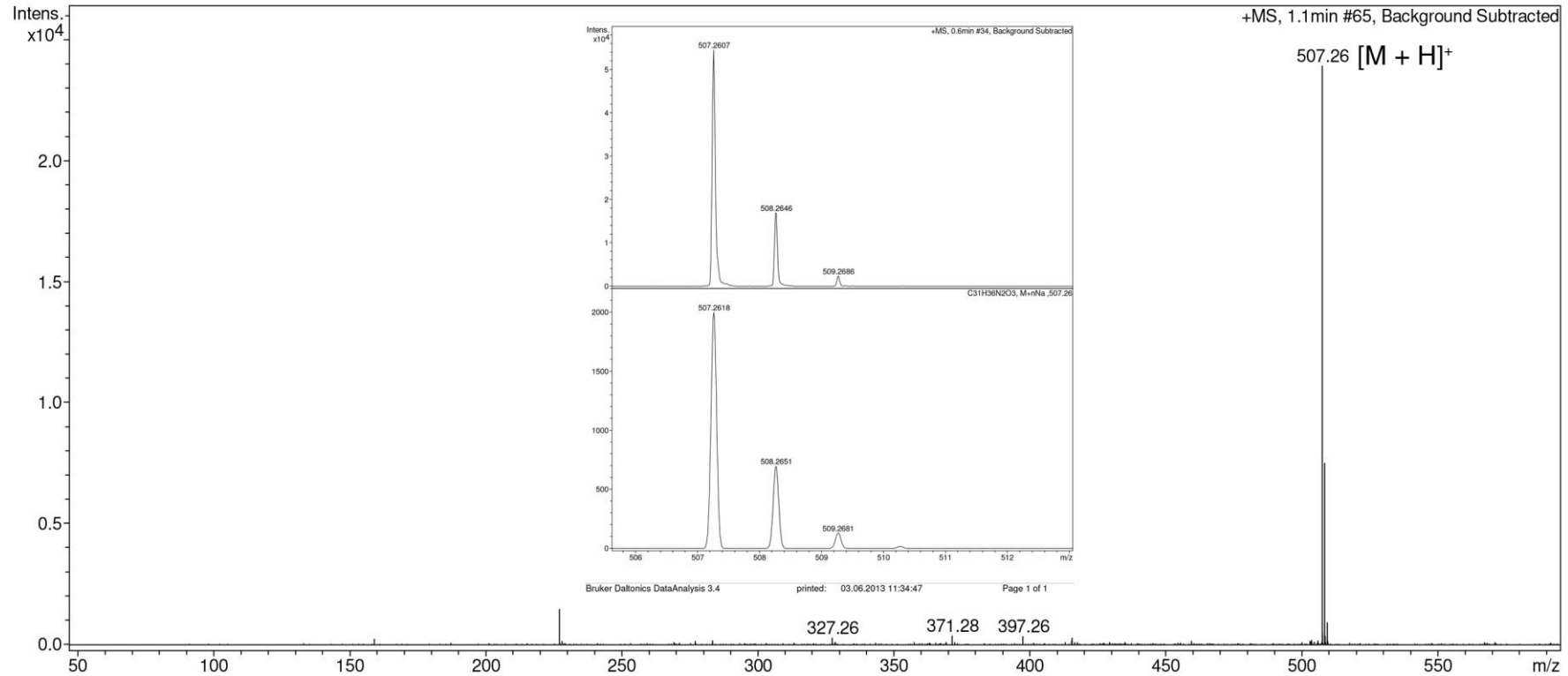
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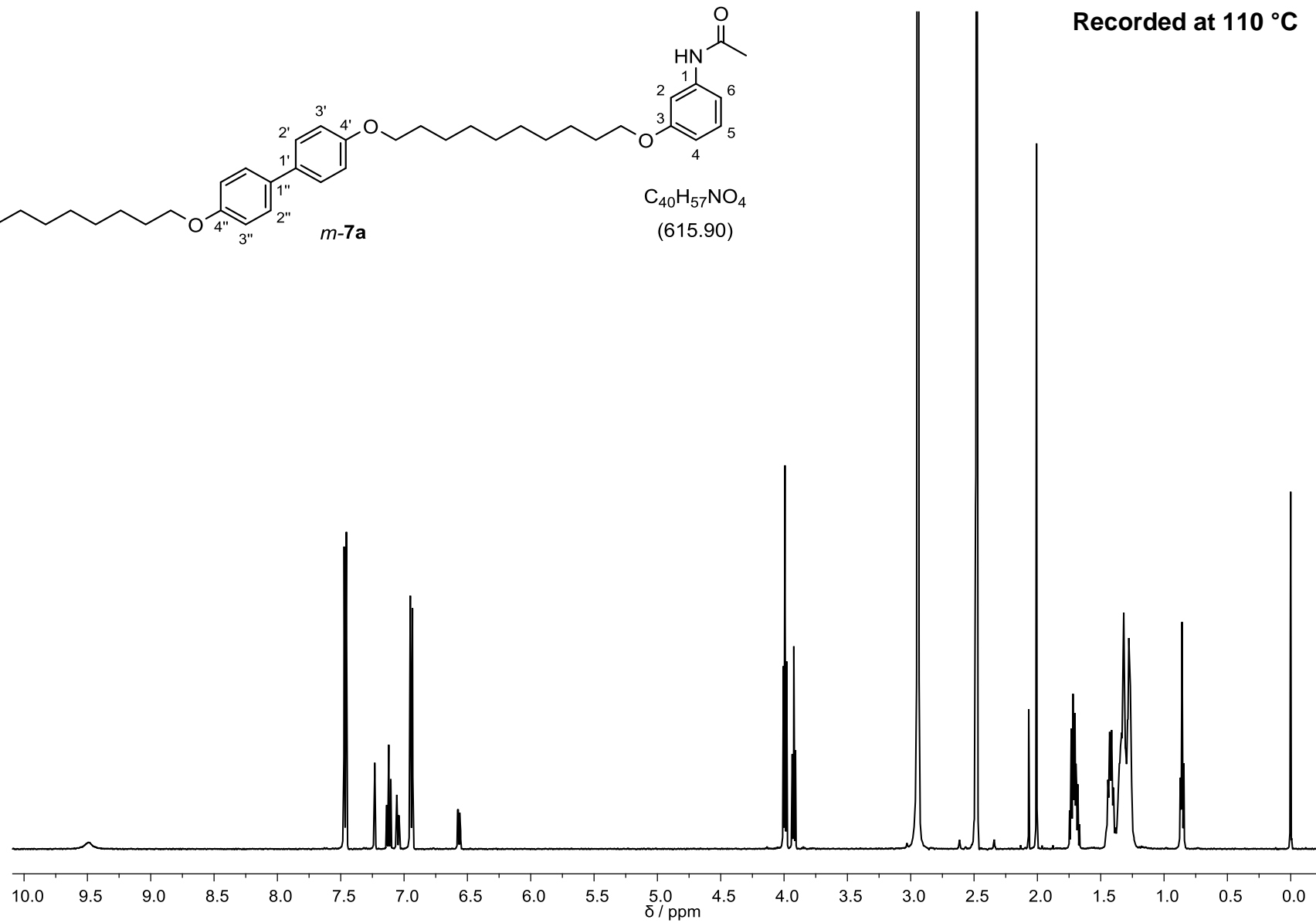
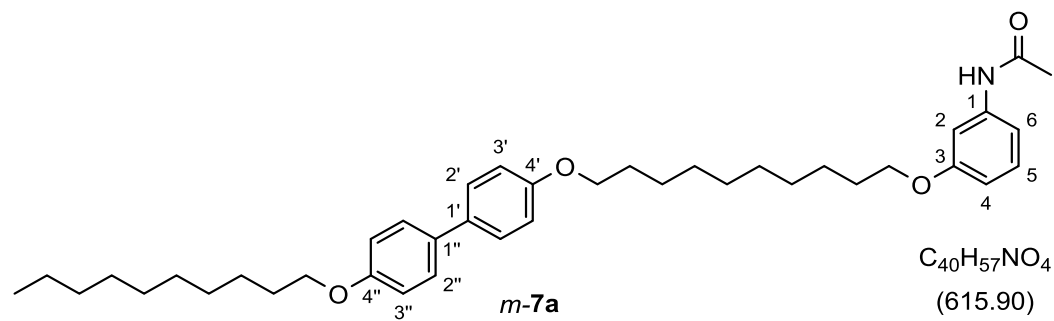
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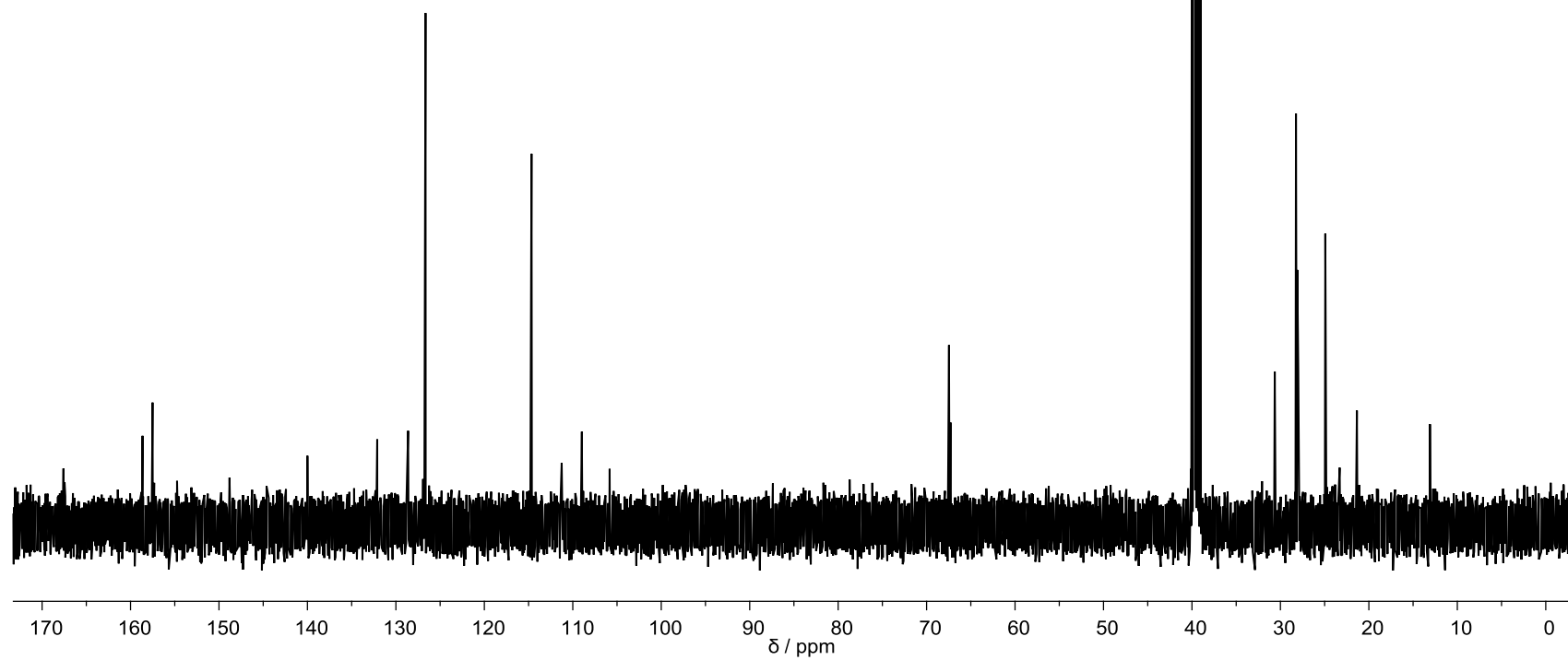
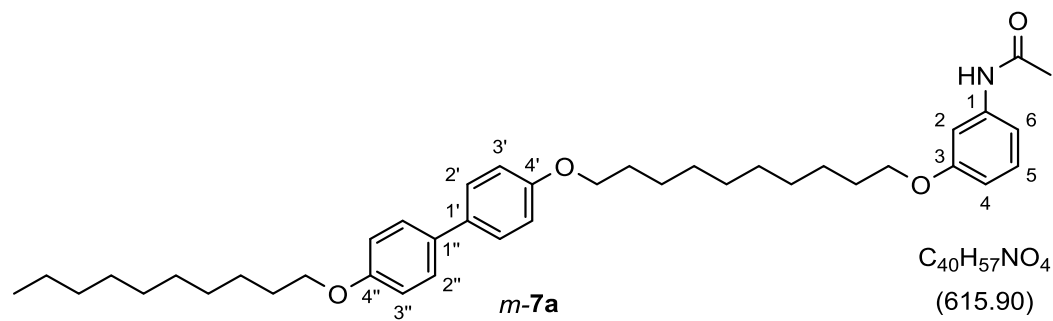
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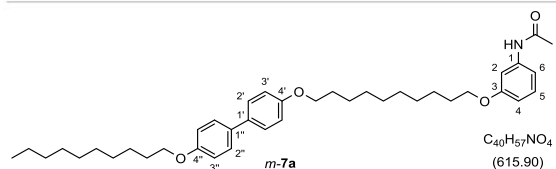
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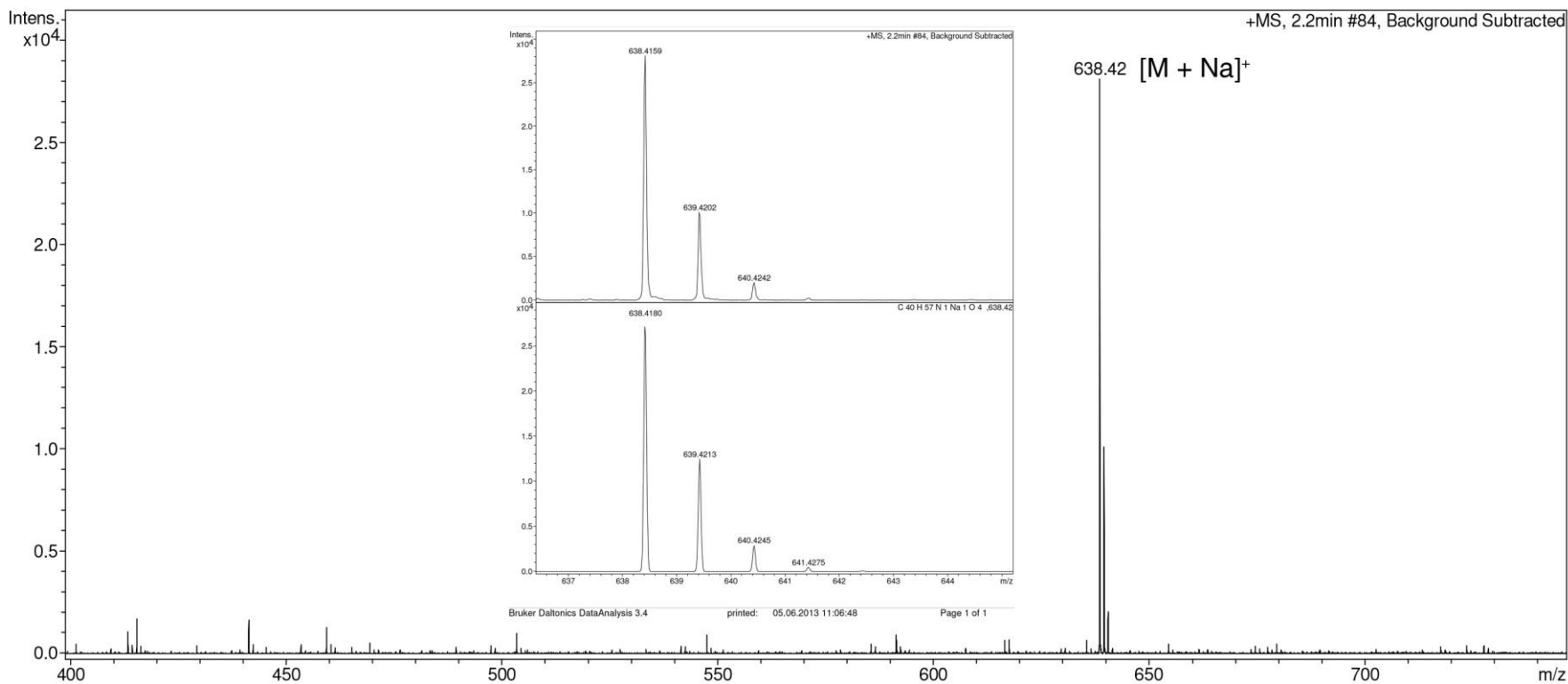
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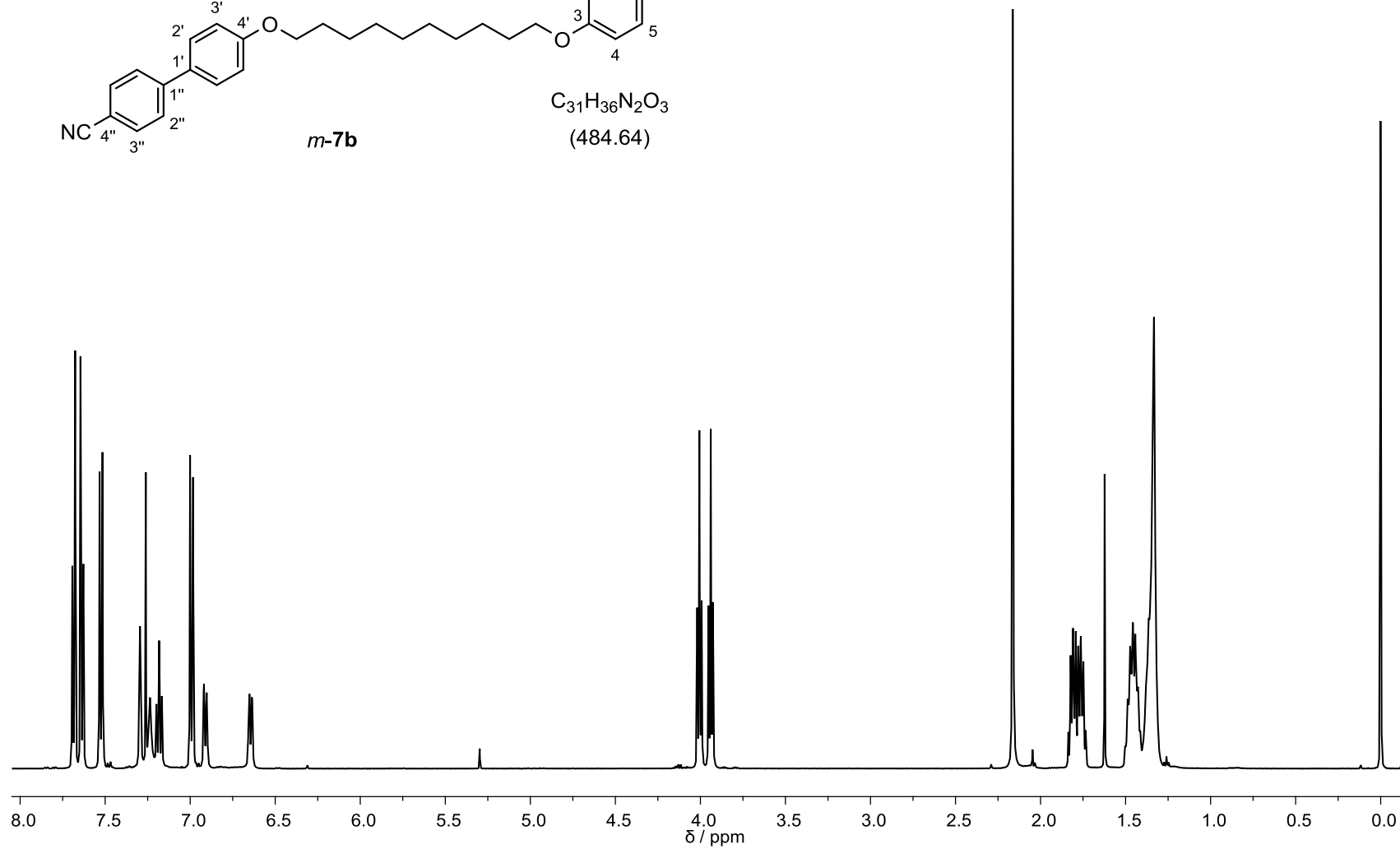
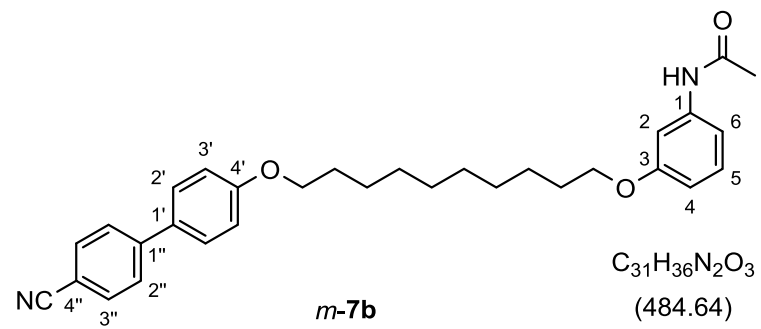


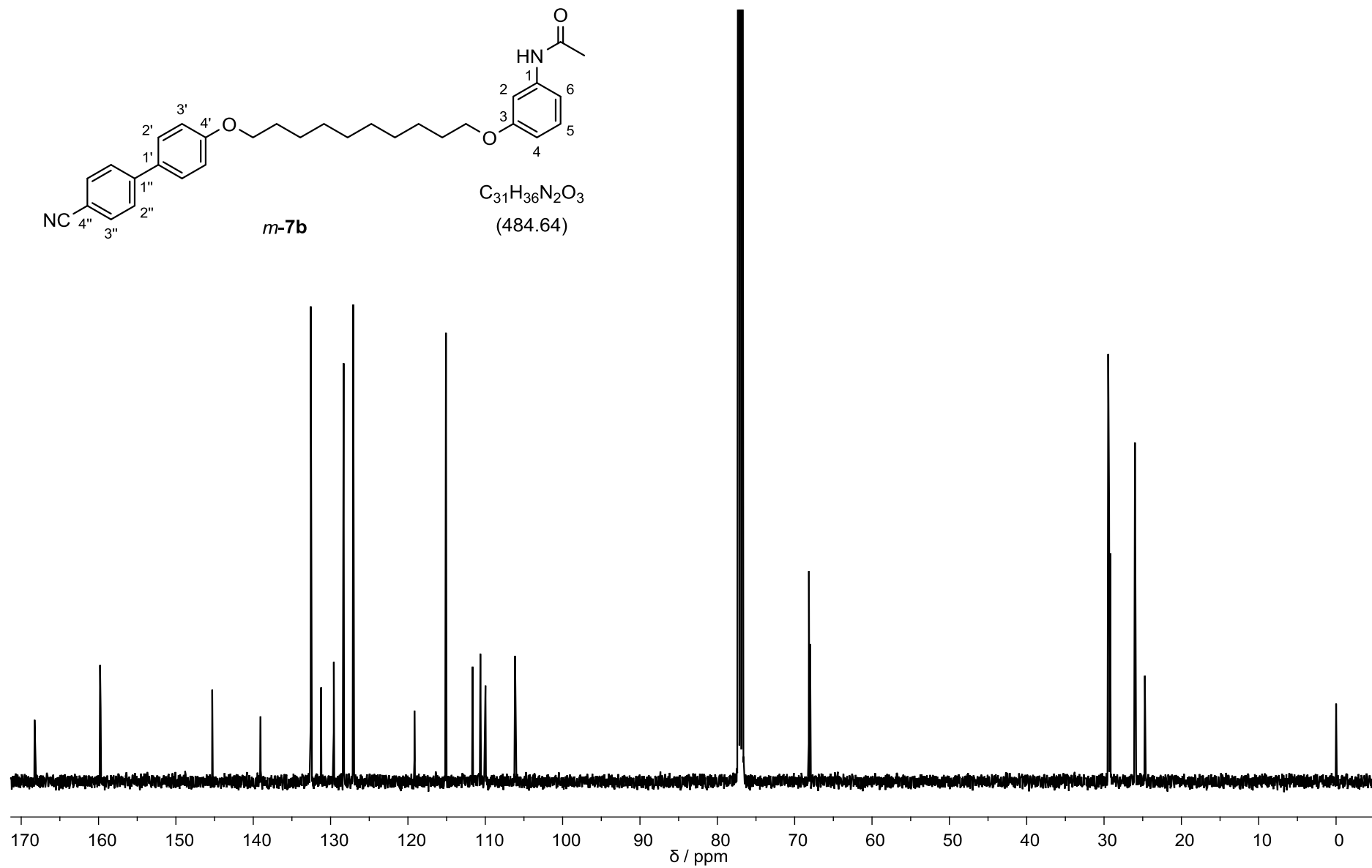
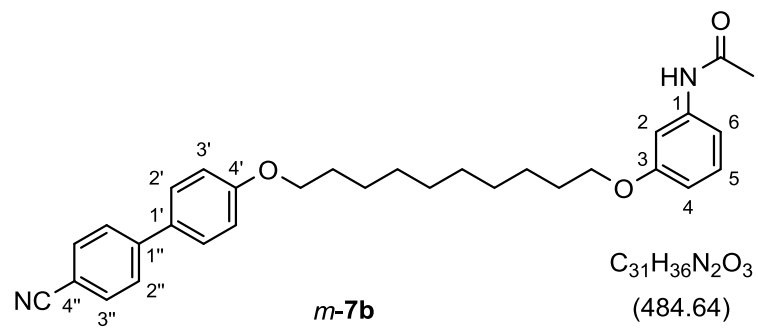
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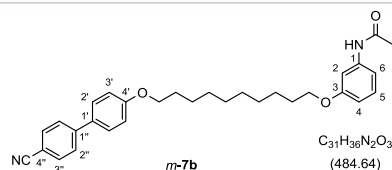
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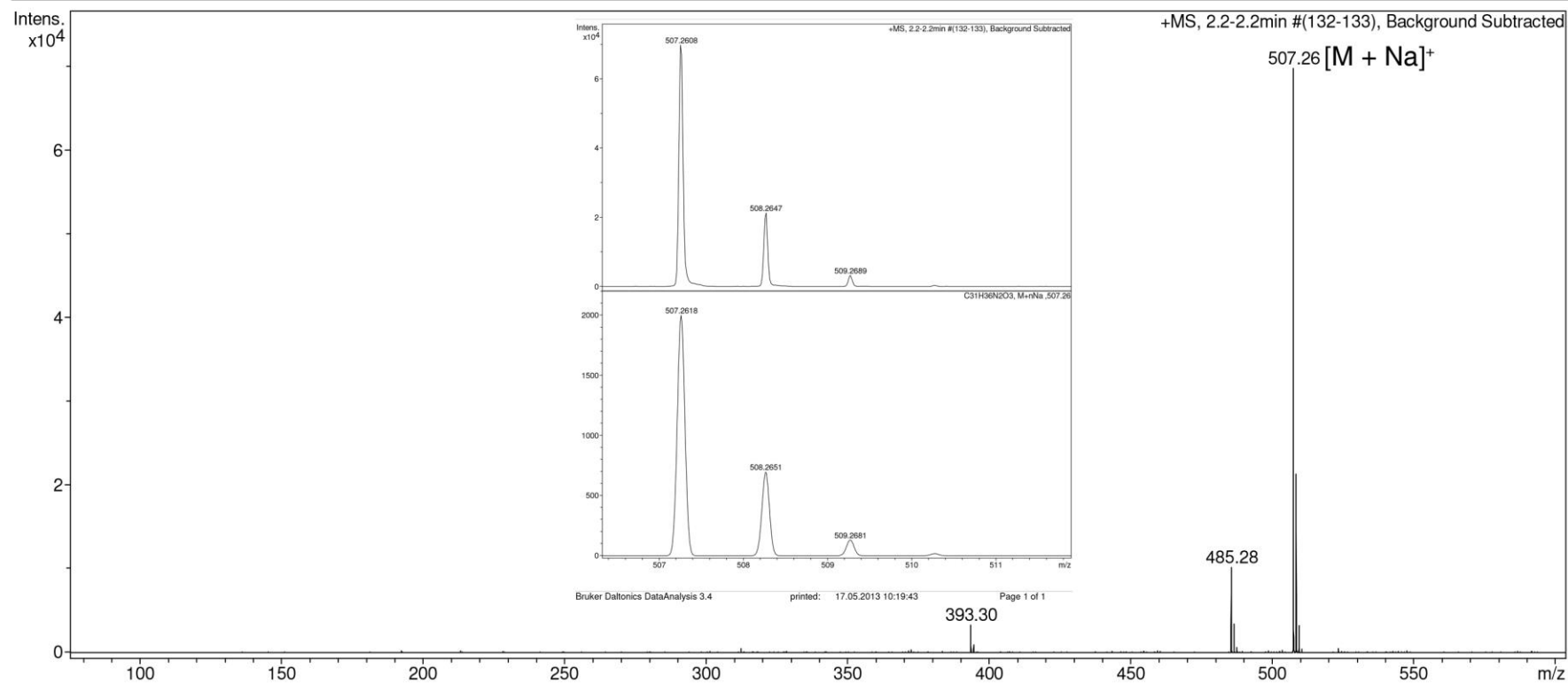
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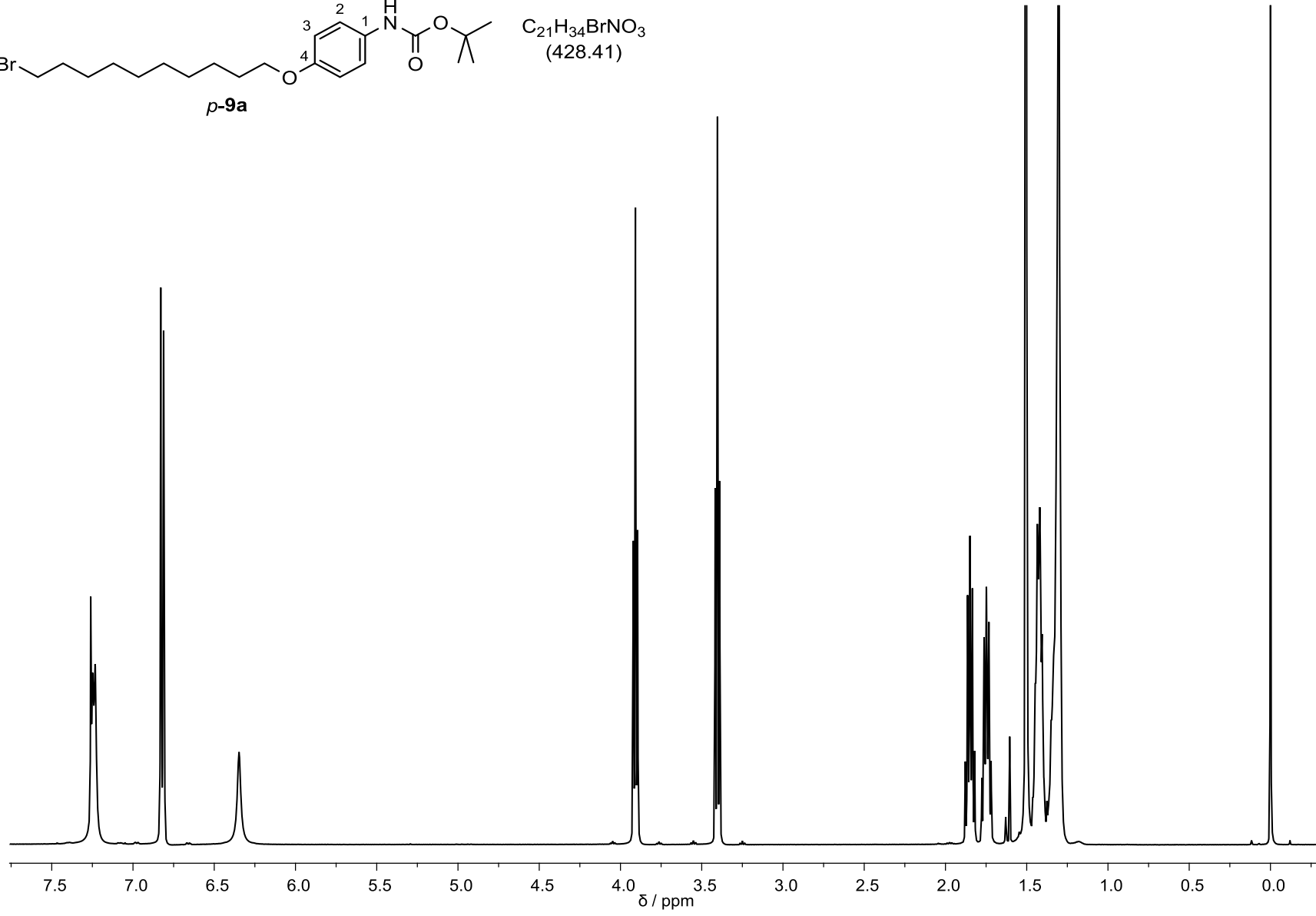
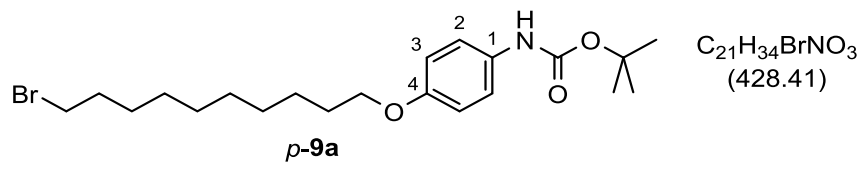


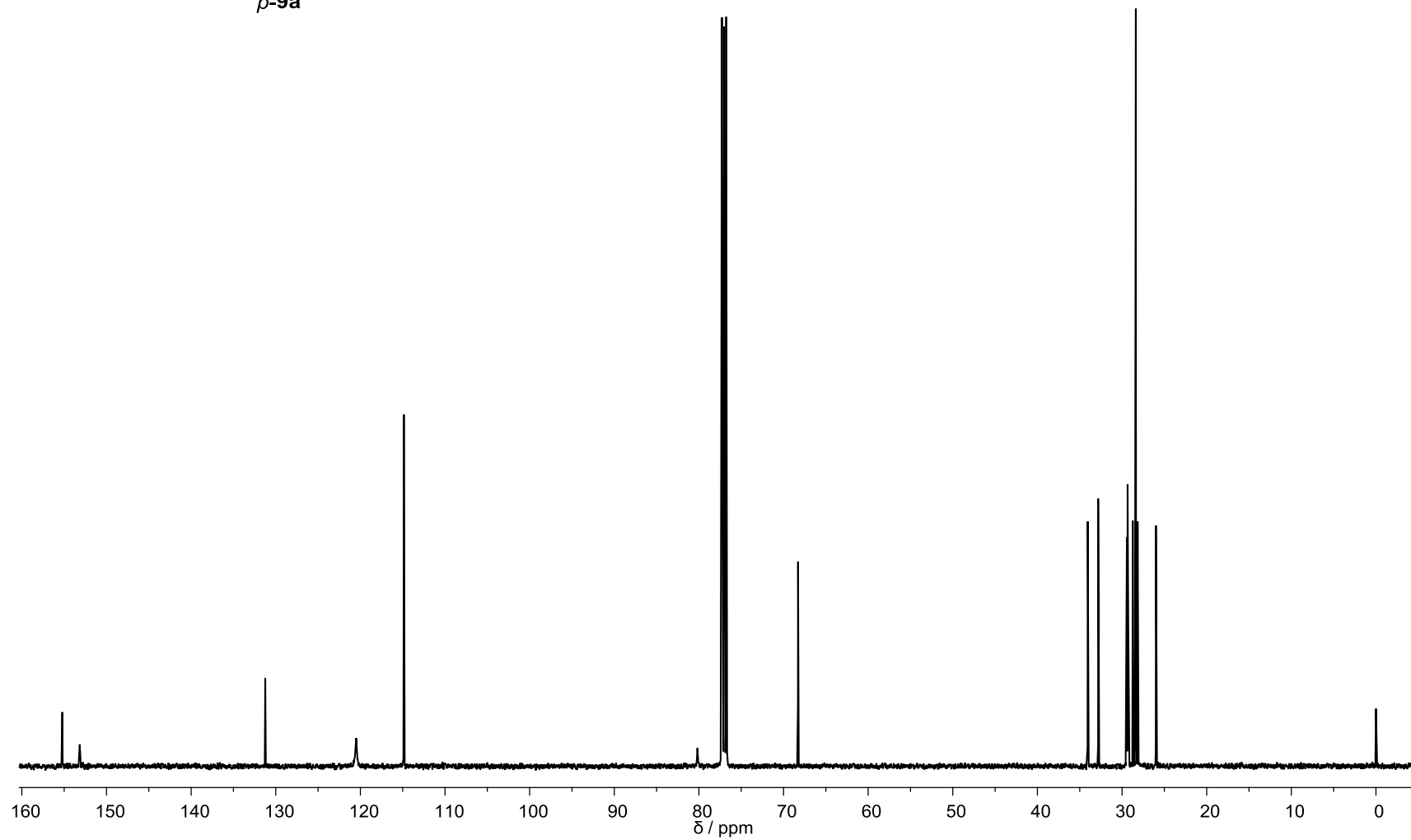
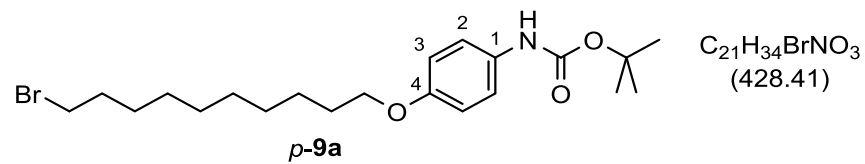
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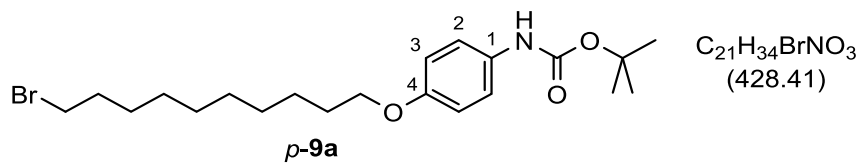
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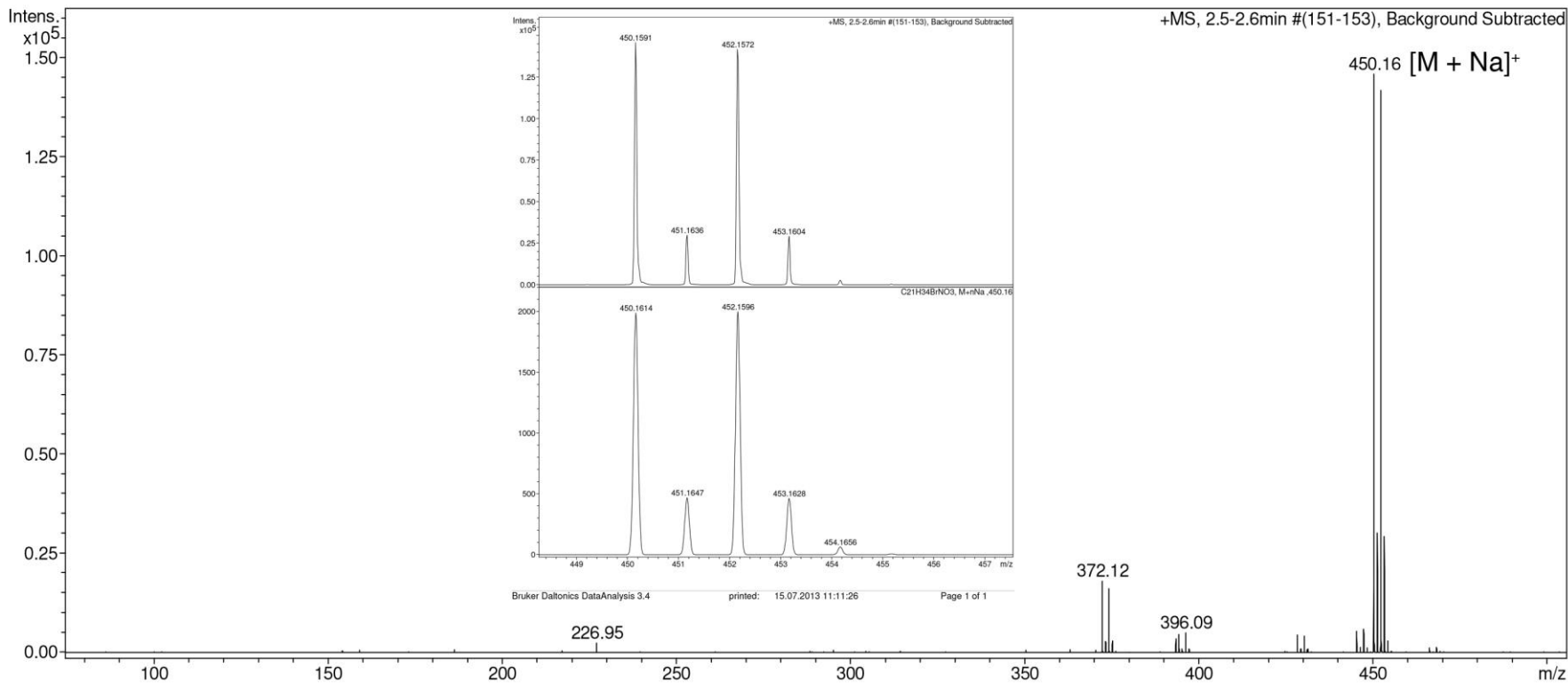
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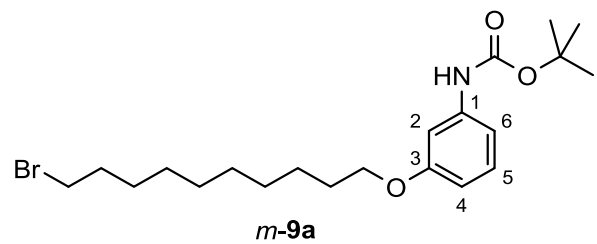


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 Instrument: micrOTOF-Q 43

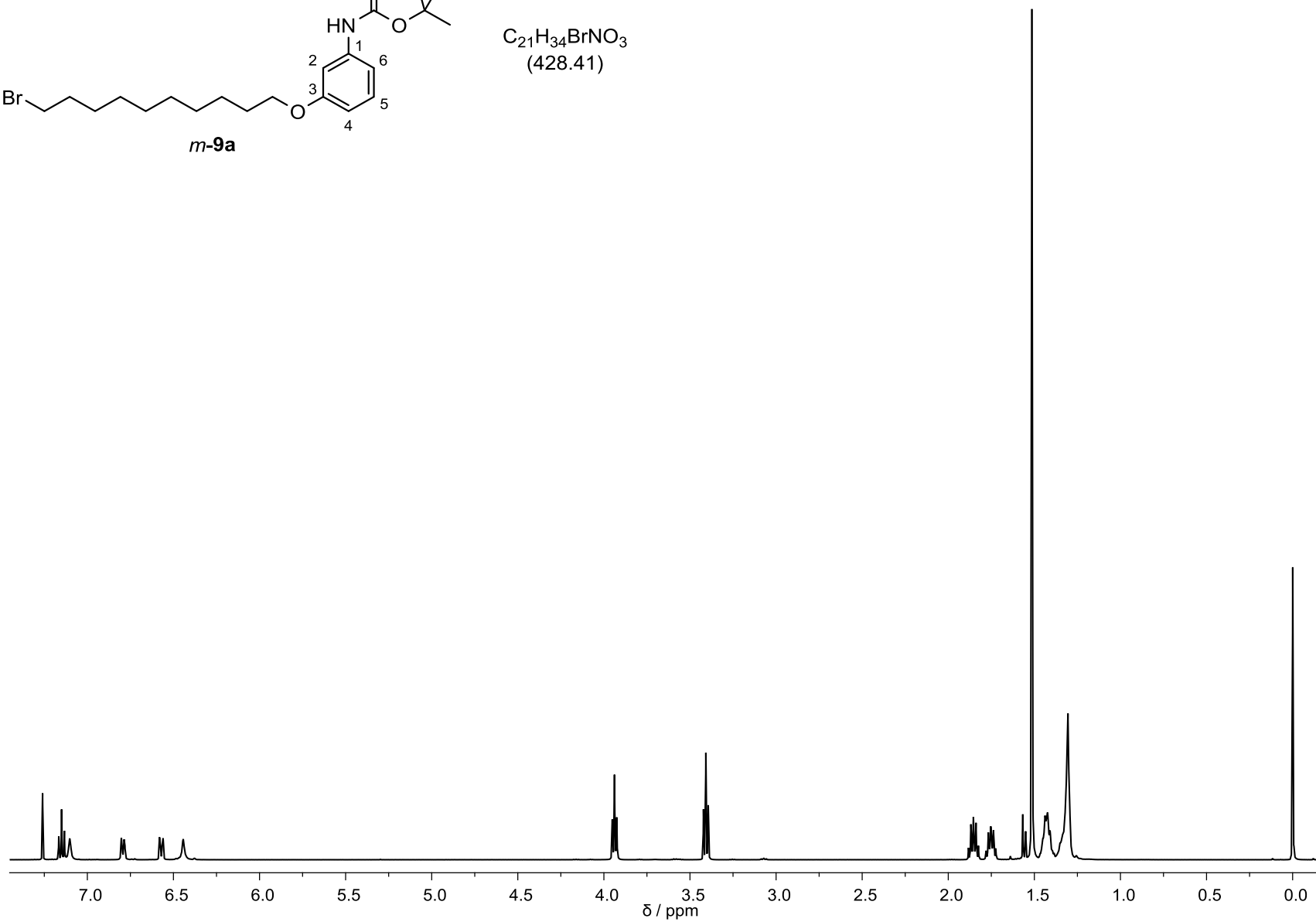
Acquisition Parameter

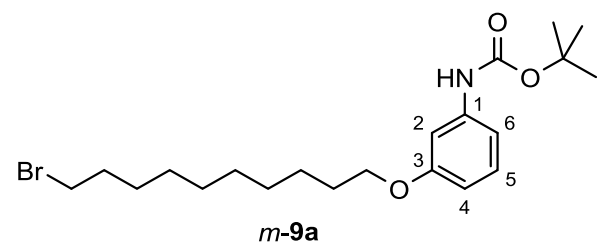
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



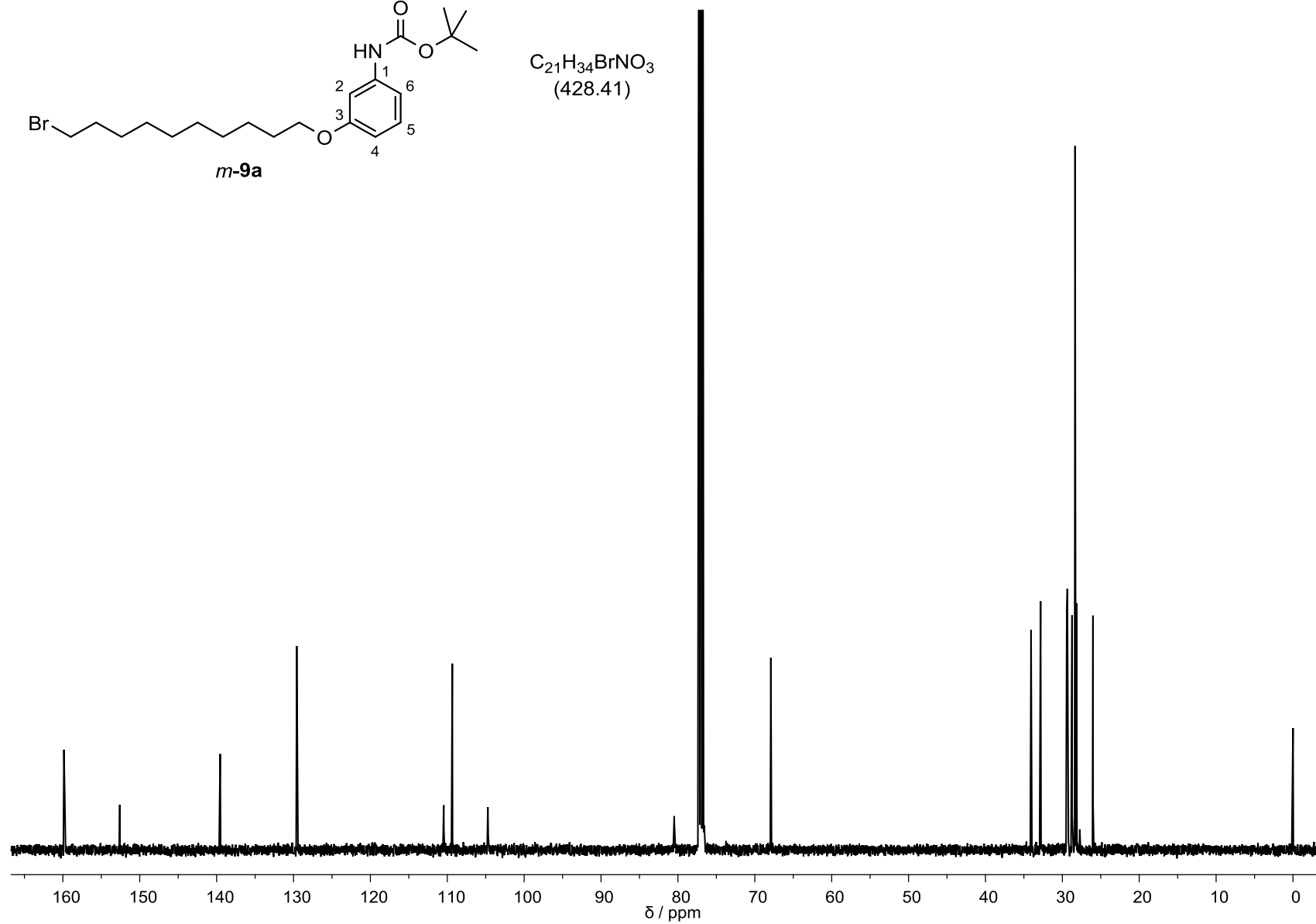


$C_{21}H_{34}BrNO_3$
(428.41)

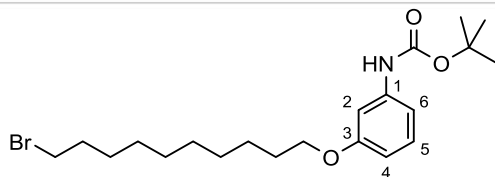




$C_{21}H_{34}BrNO_3$
(428.41)



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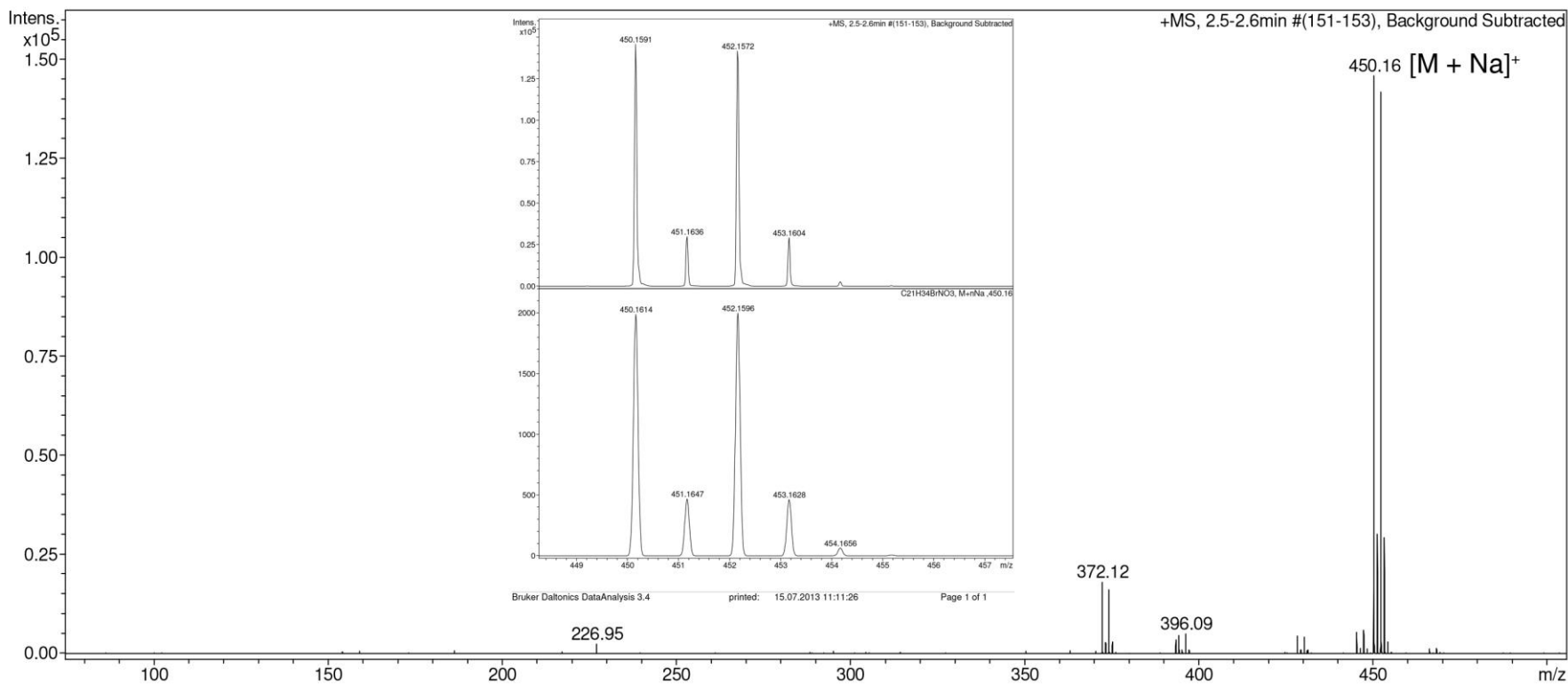


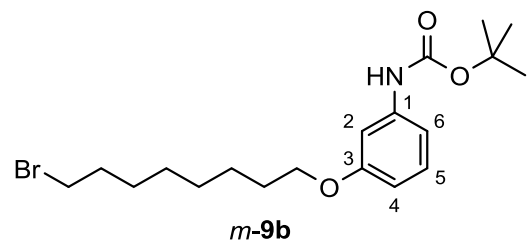
$C_{21}H_{34}BrNO_3$
(428.41)

Acquisition Date 15.07.2013 10:30:04
Operator wo/tri
Instrument micrOTOF-Q 43

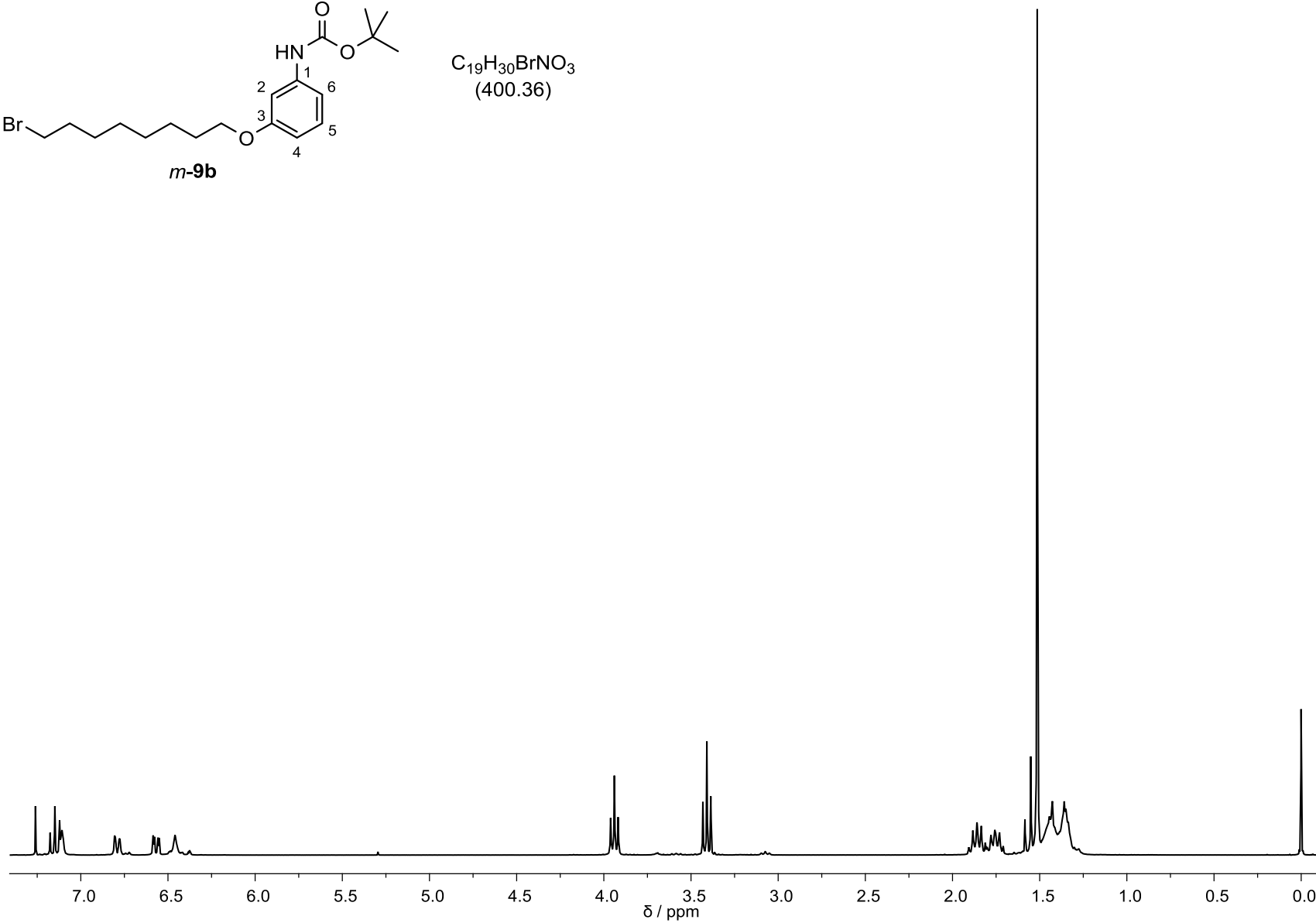
Acquisition Parameter 21-9a

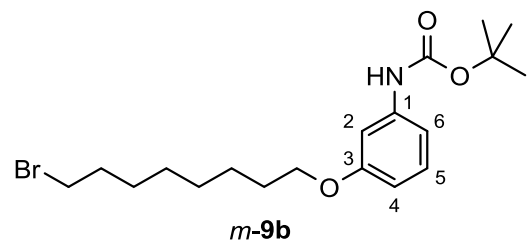
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Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



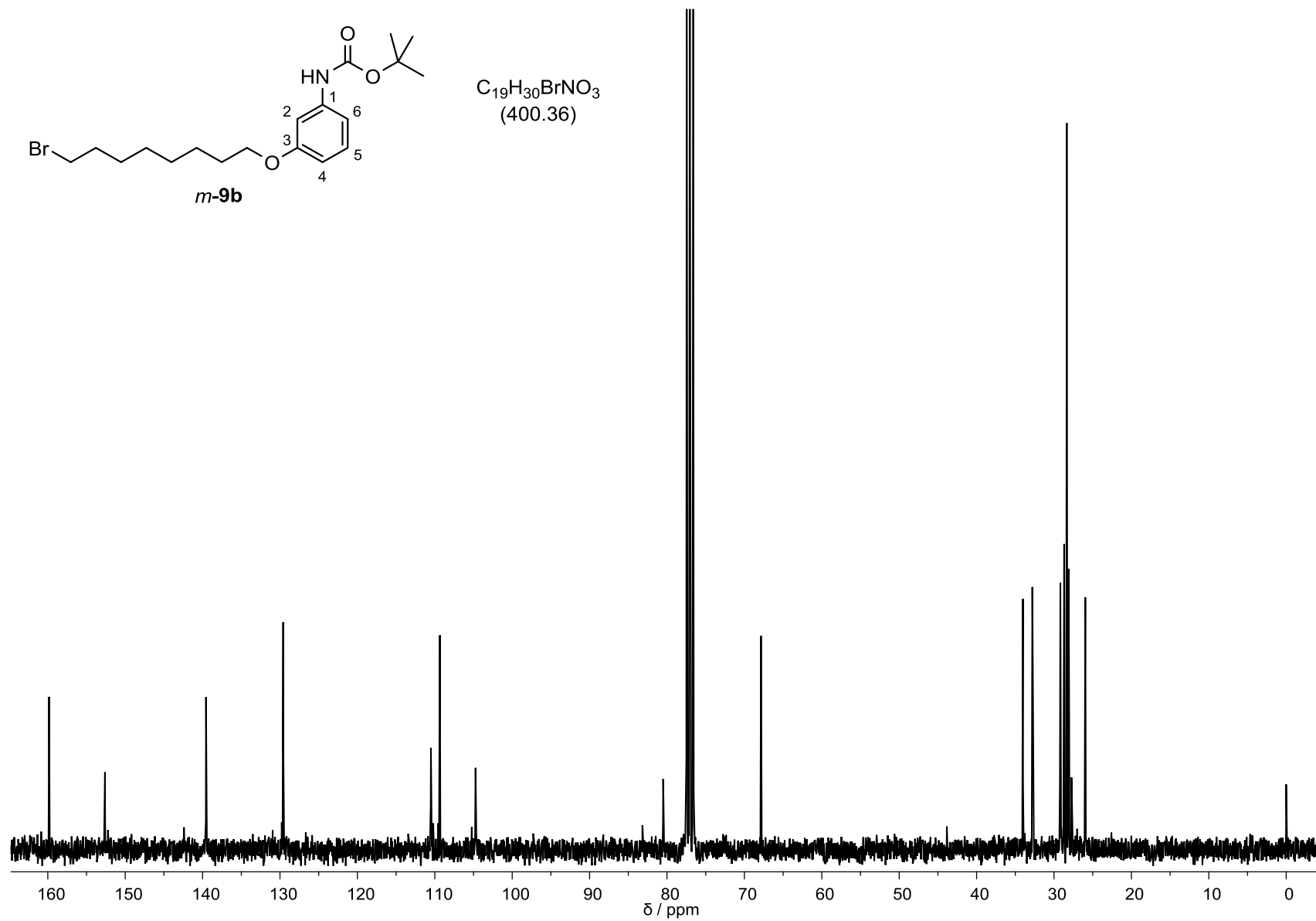


$C_{19}H_{30}BrNO_3$
(400.36)

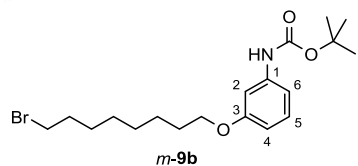




$C_{19}H_{30}BrNO_3$
(400.36)



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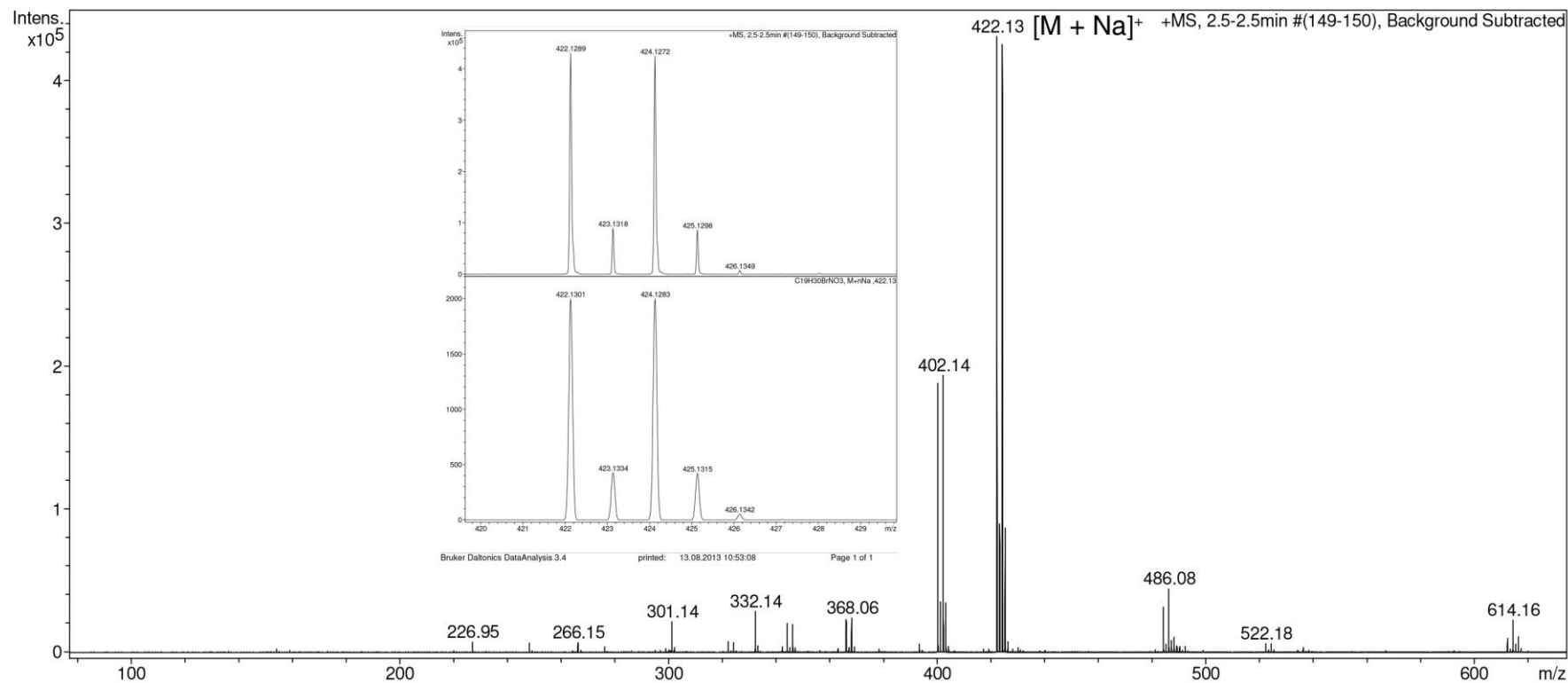


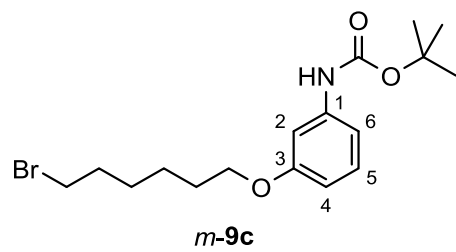
$C_{19}H_{30}BrNO_3$
(400.36)

Acquisition Date 13.08.2013 09:22:30
Operator wo/tri
Instrument micrOTOF-Q 43

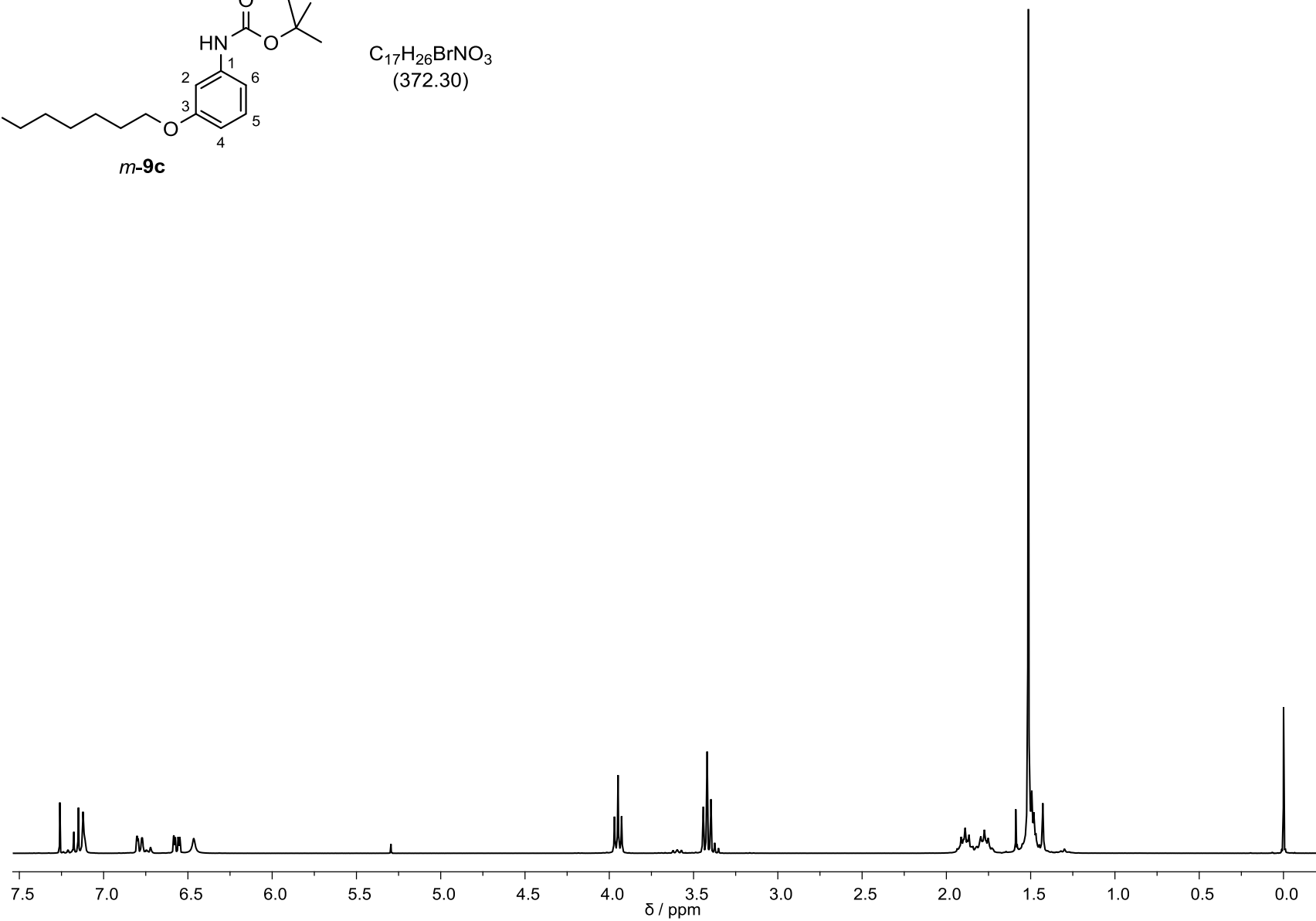
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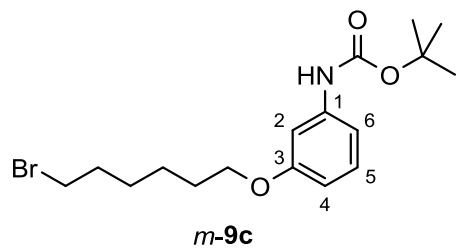
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



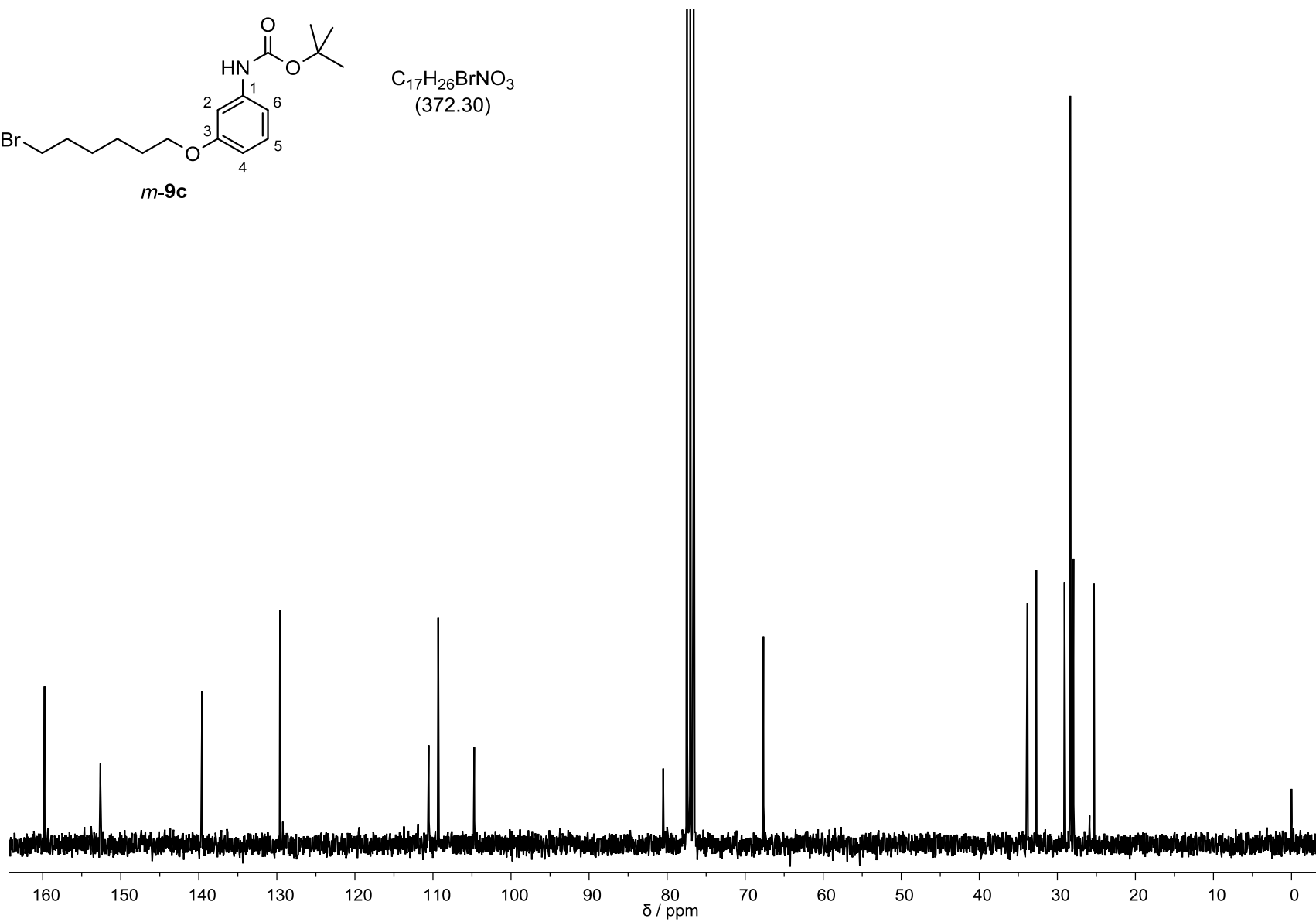


C₁₇H₂₆BrNO₃
(372.30)

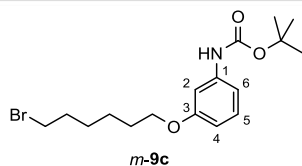




C₁₇H₂₆BrNO₃
(372.30)



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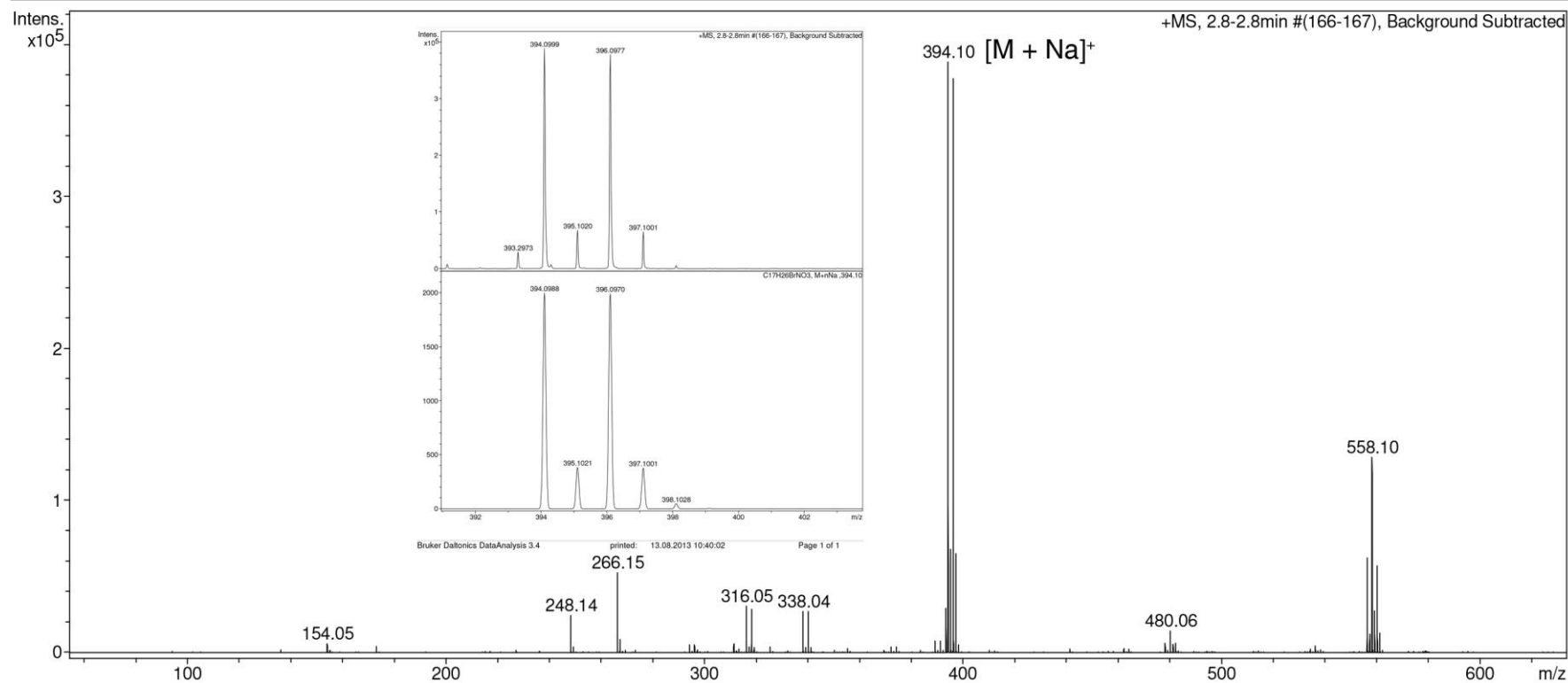


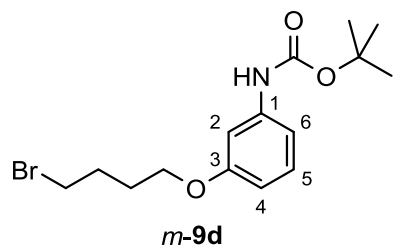
C₁₇H₂₆BrNO₃
(372.30)

Acquisition Date 13.08.2013 09:16:26
Operator wo/tri
Instrument micrOTOF-Q 43

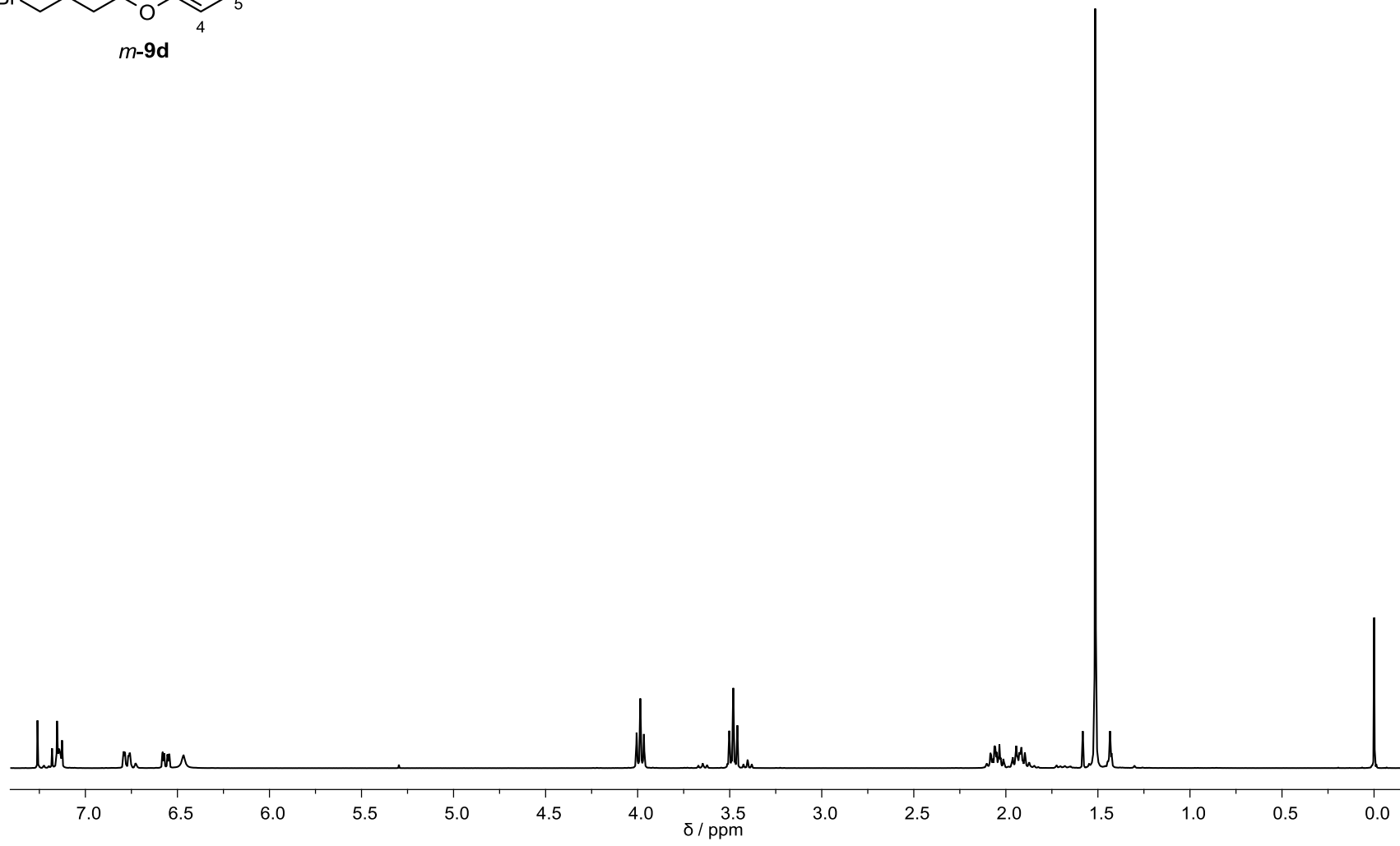
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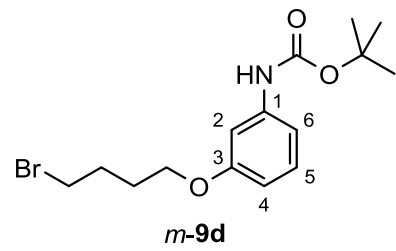
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Scan End	1000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste



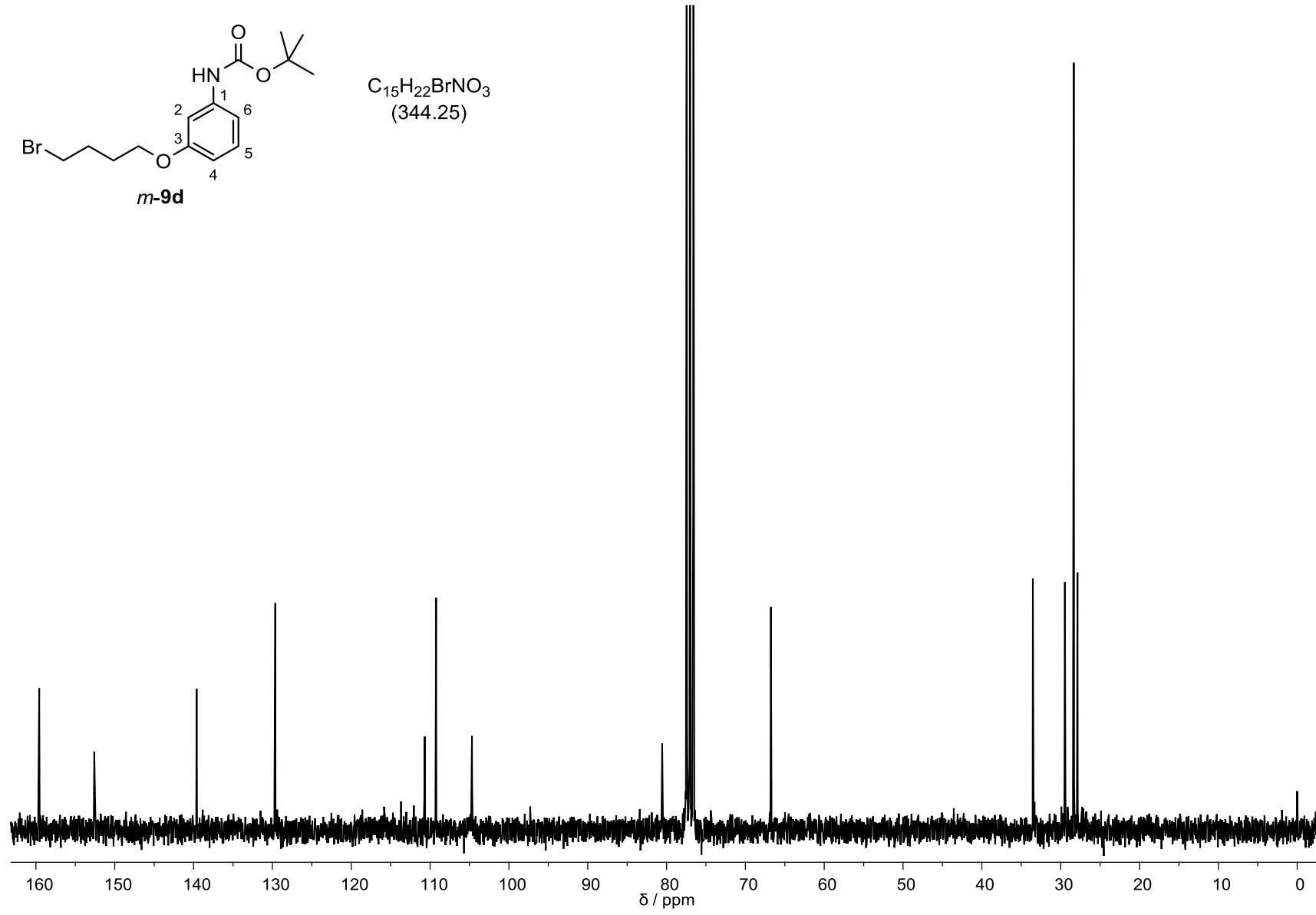


$C_{15}H_{22}BrNO_3$
(344.25)

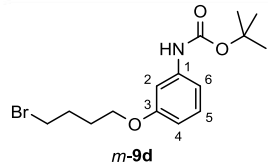




$C_{15}H_{22}BrNO_3$
(344.25)



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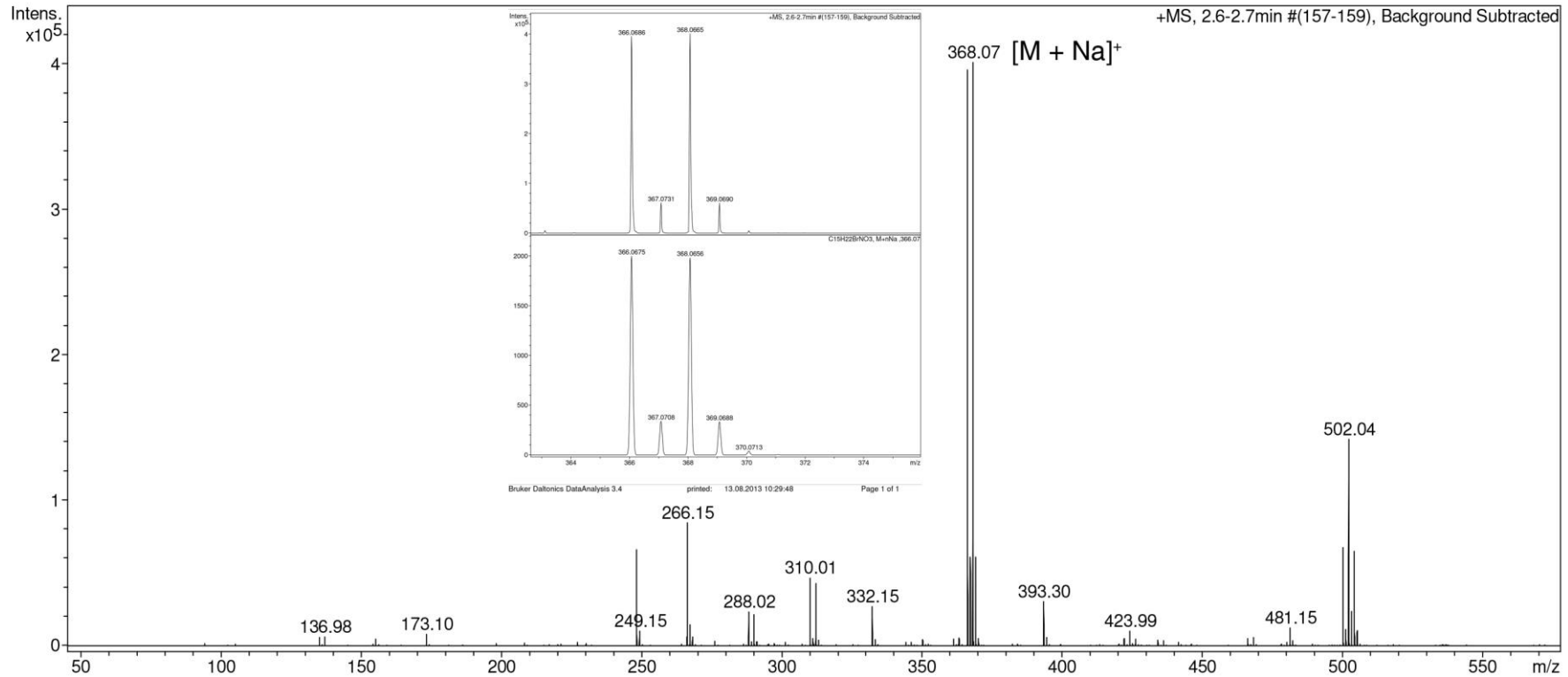
C₁₅H₂₂BrNO₃
(344.25)

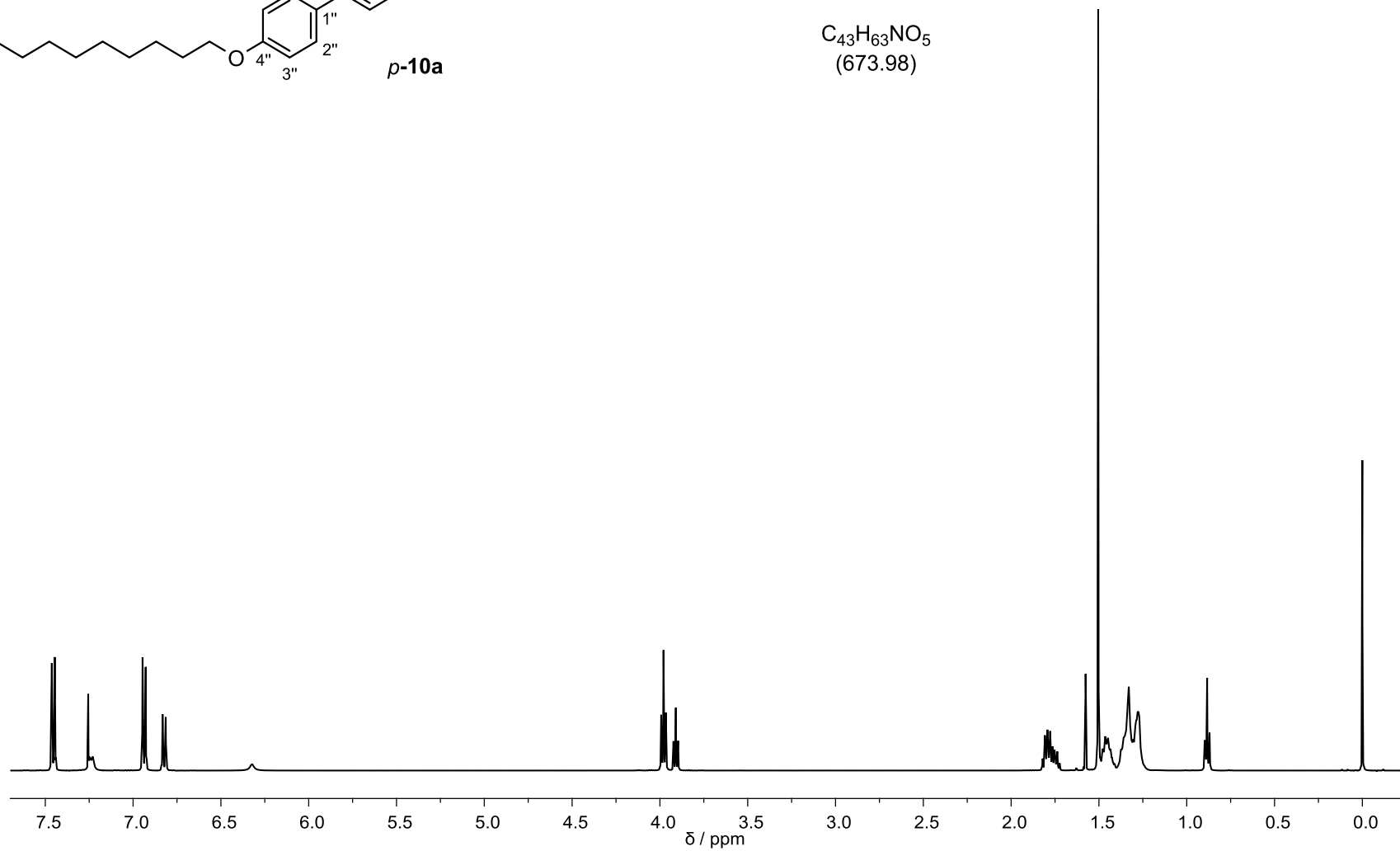
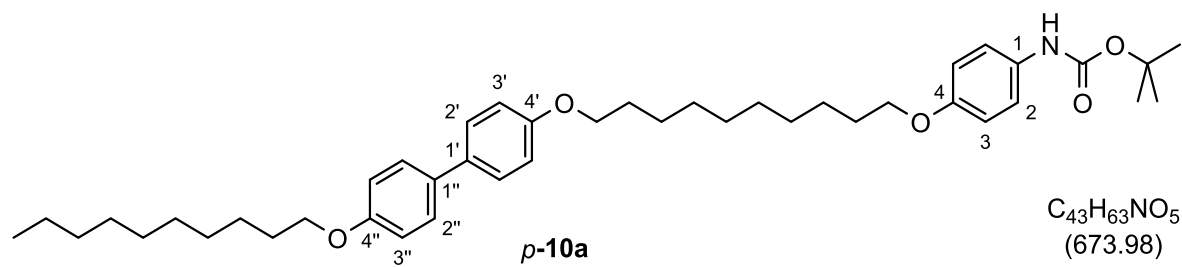
Acquisition Date 13.08.2013 09:10:15

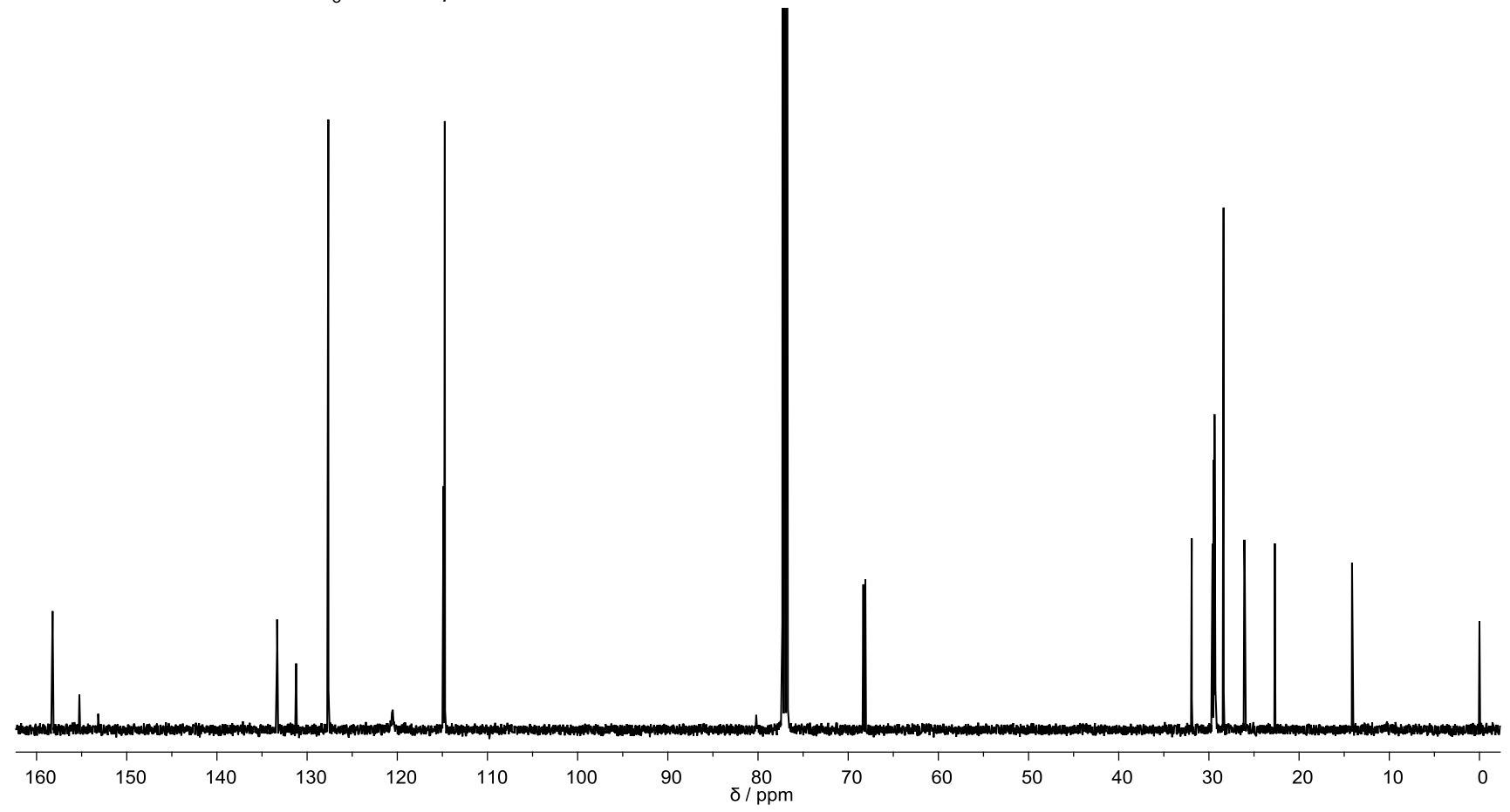
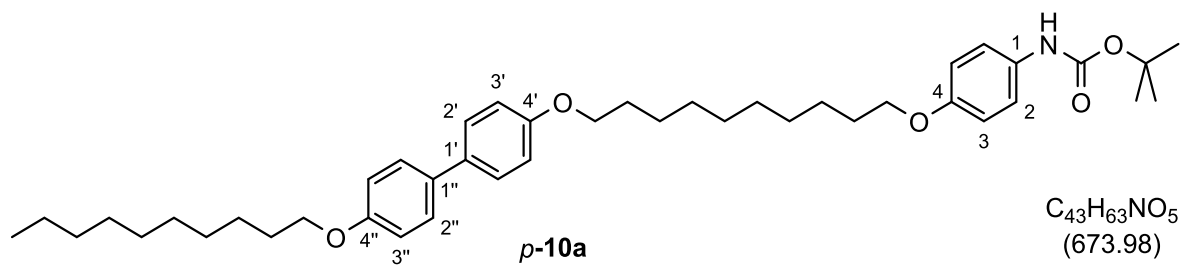
Operator wo/tri
Instrument micrOTOF-Q 43

Acquisition Parameter

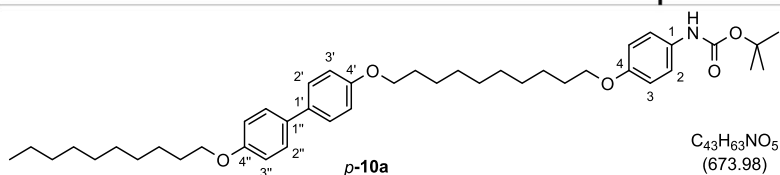
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Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
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Scan End	1000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste







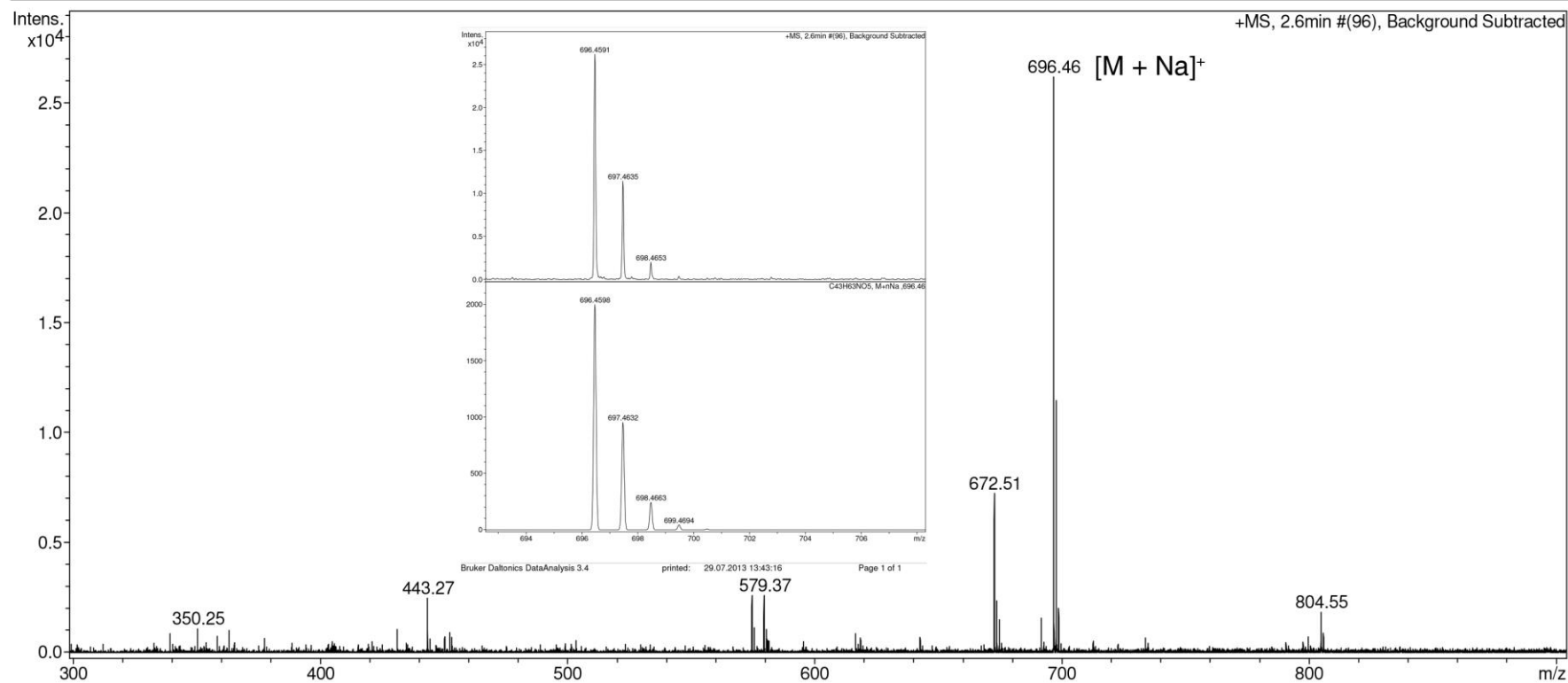
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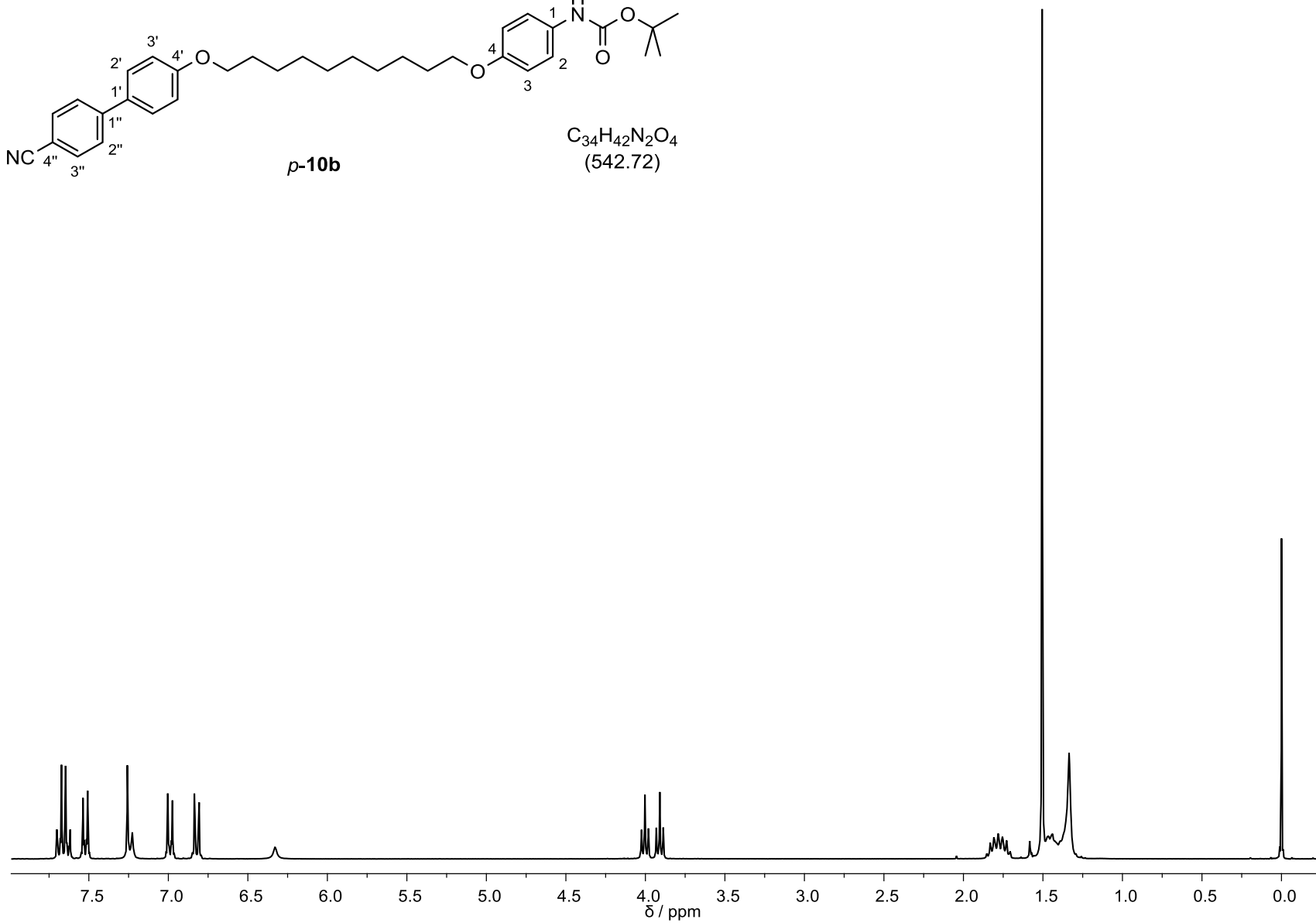
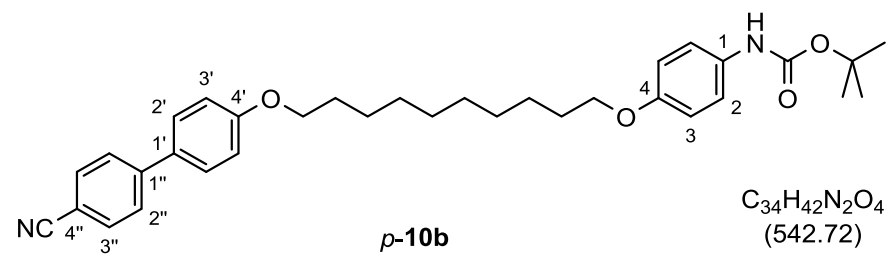


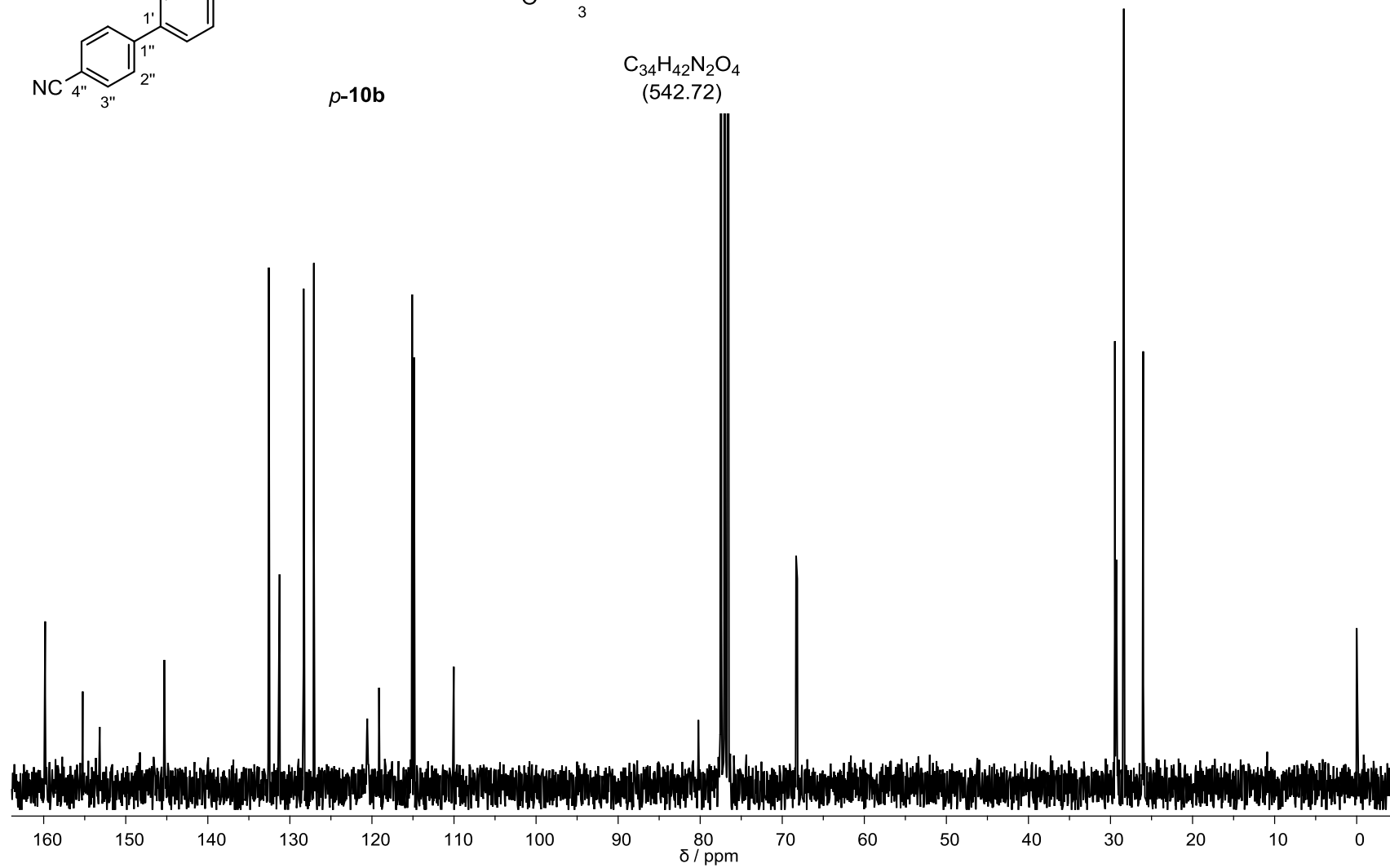
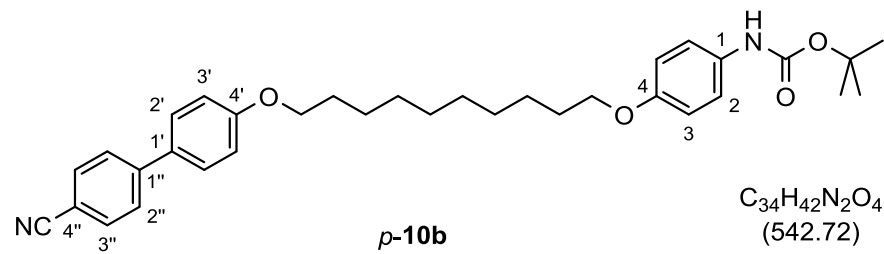
Acquisition Date 29.07.2013 11:34:54
 Operator wo/tri
 Instrument micrOTOF-Q 43

Acquisition Parameter

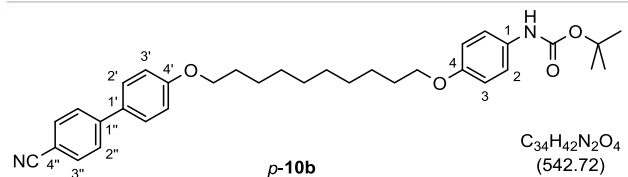
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Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	200 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste







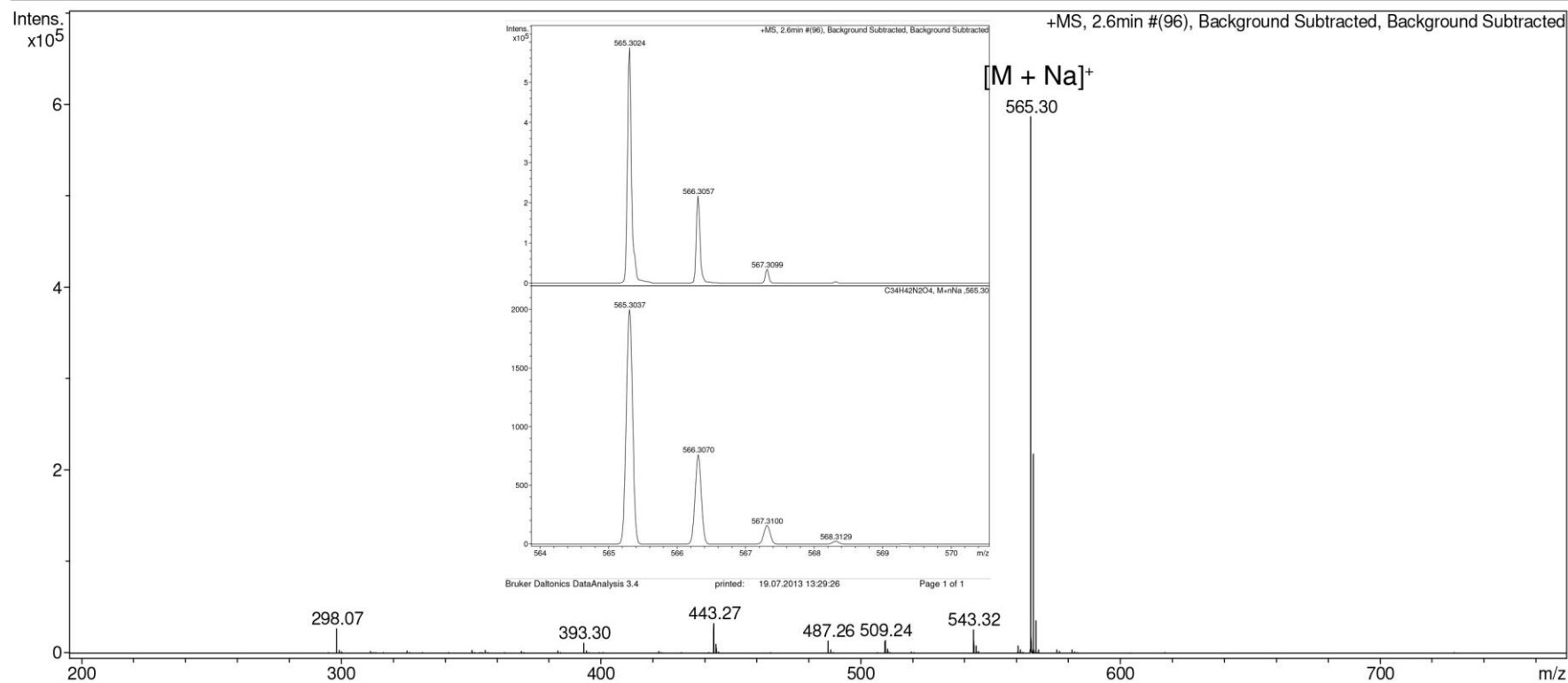
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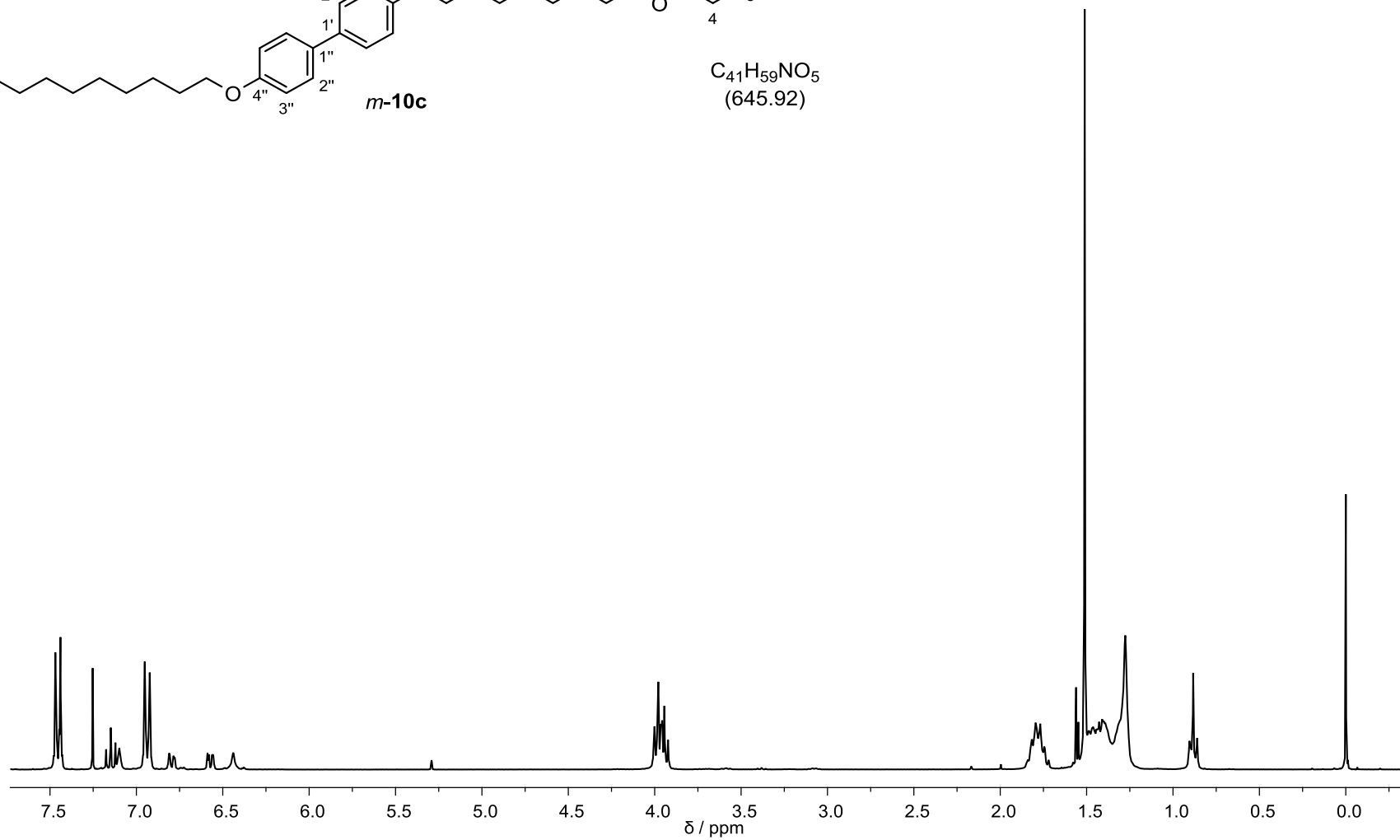
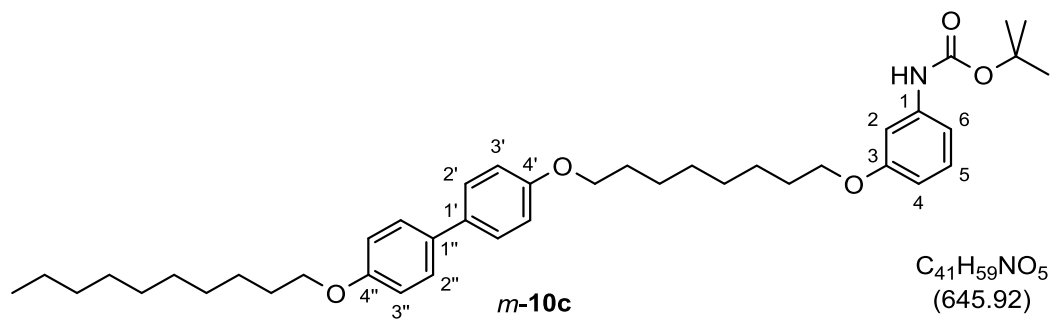


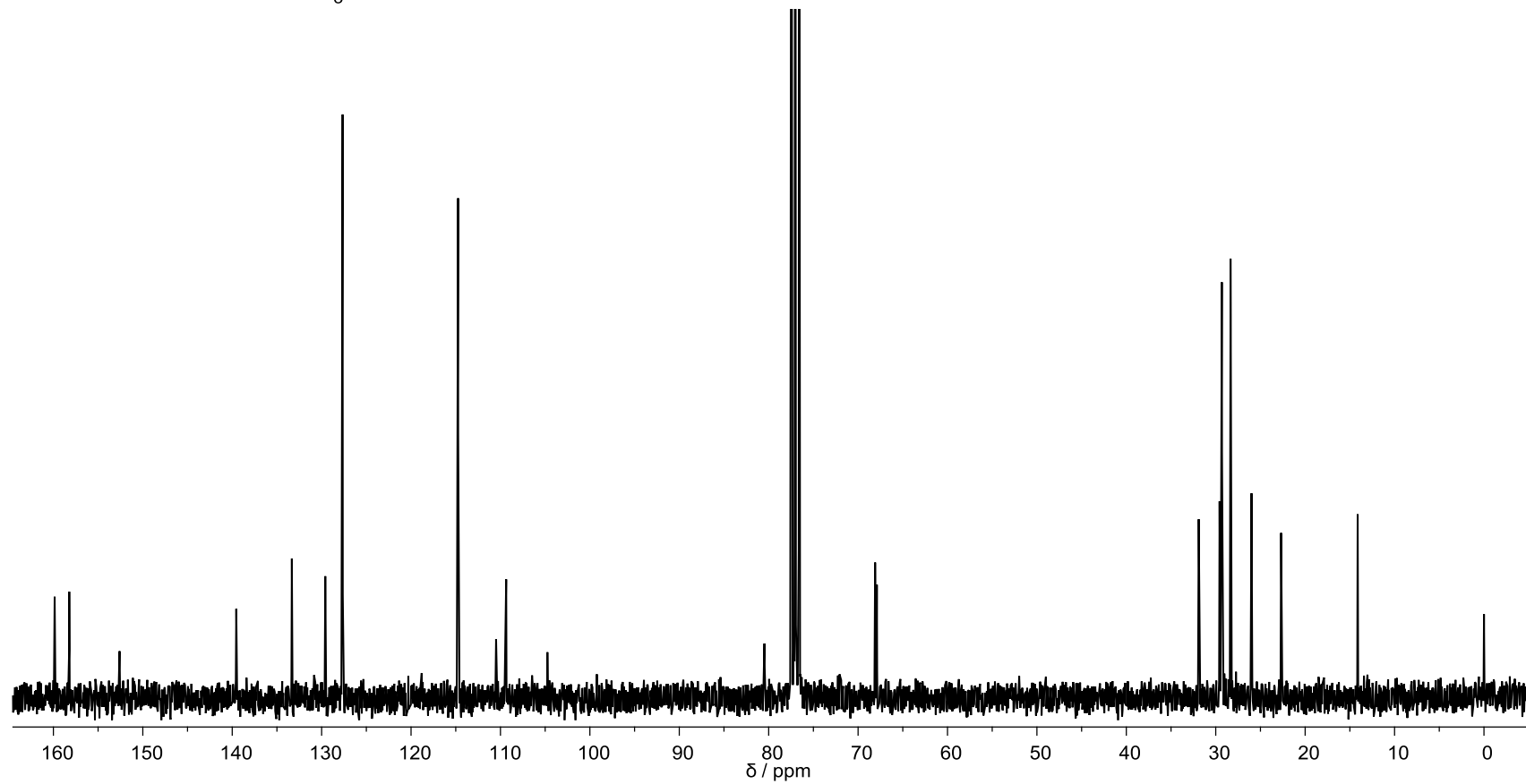
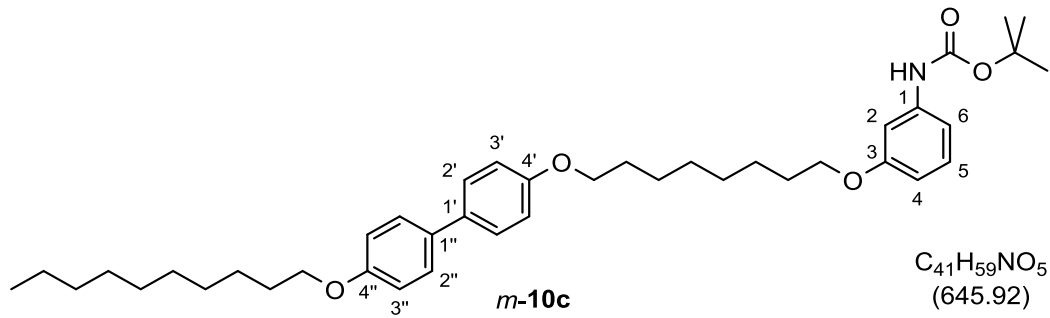
Acquisition Date 19.07.2013 11:29:16
 Operator wo/tri
 Instrument micrOTOF-Q 43

Acquisition Parameter

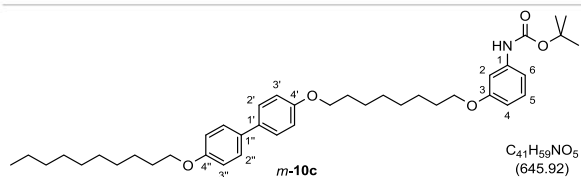
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Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
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Scan End	2500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste







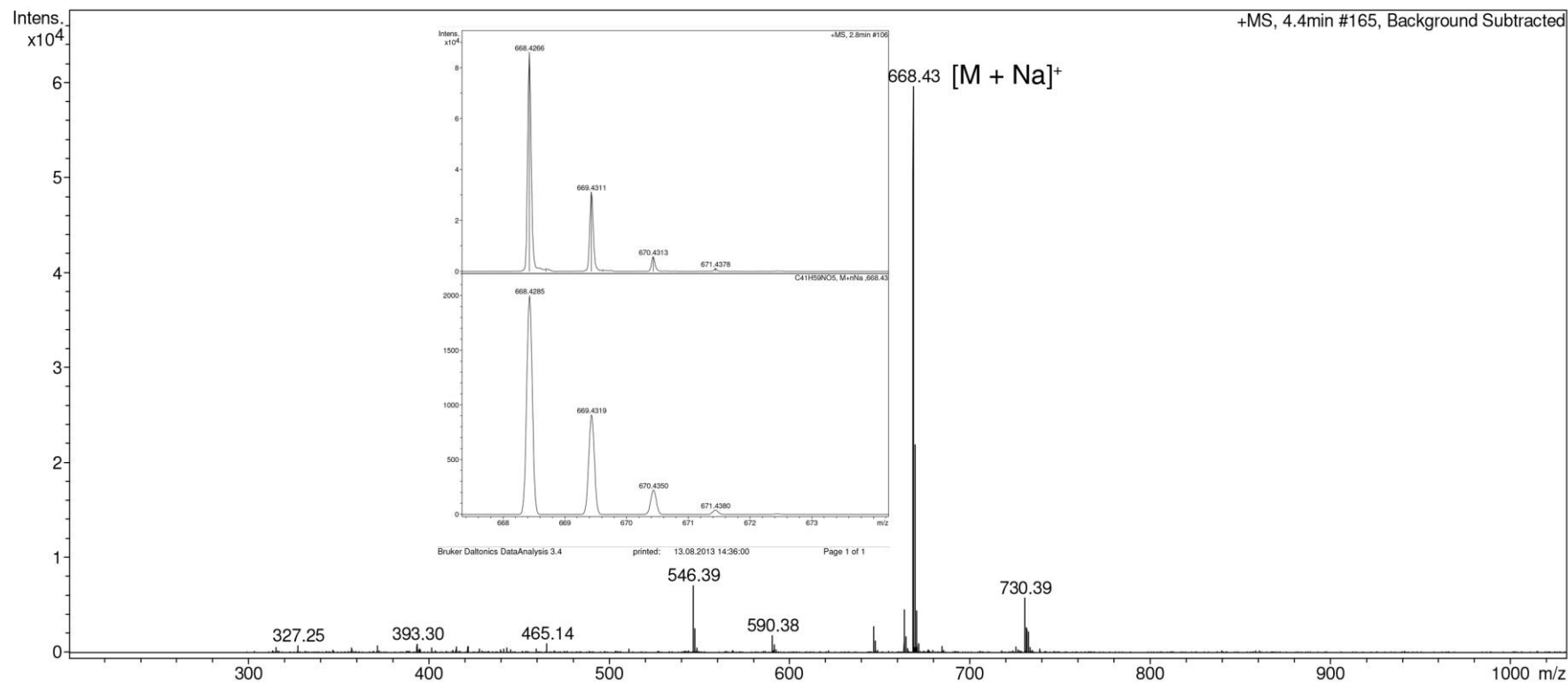
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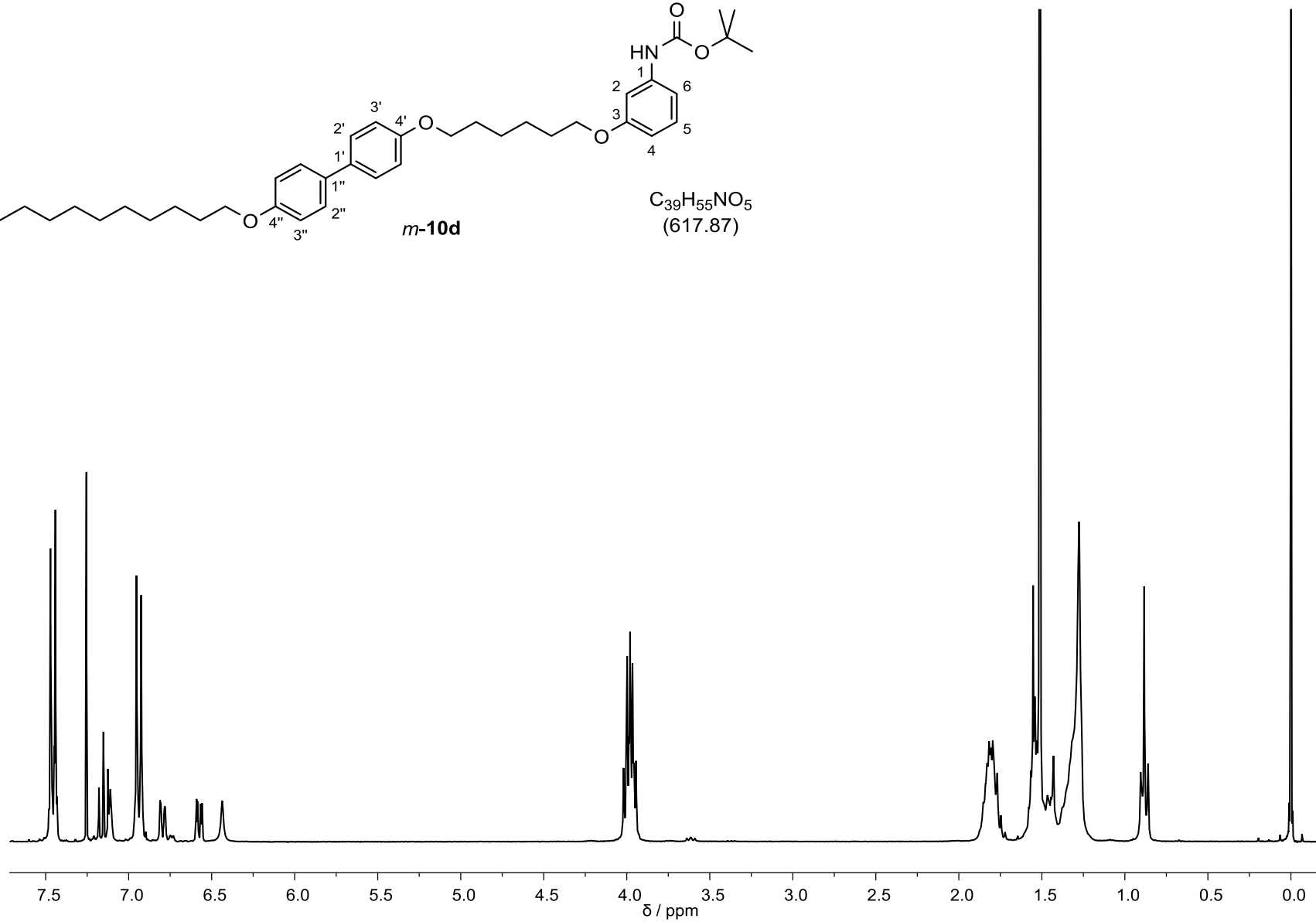
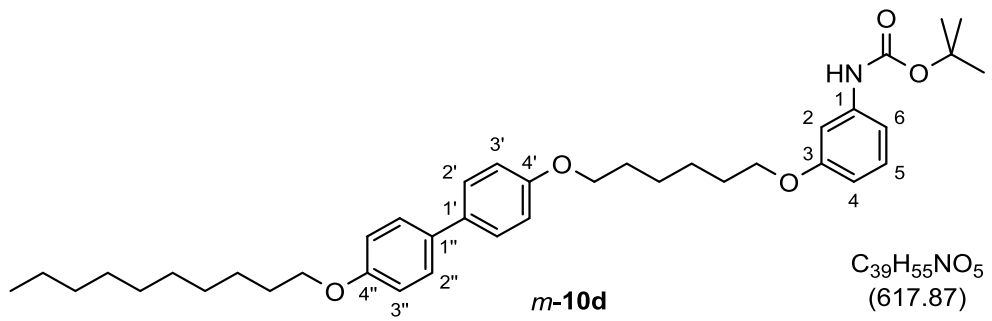


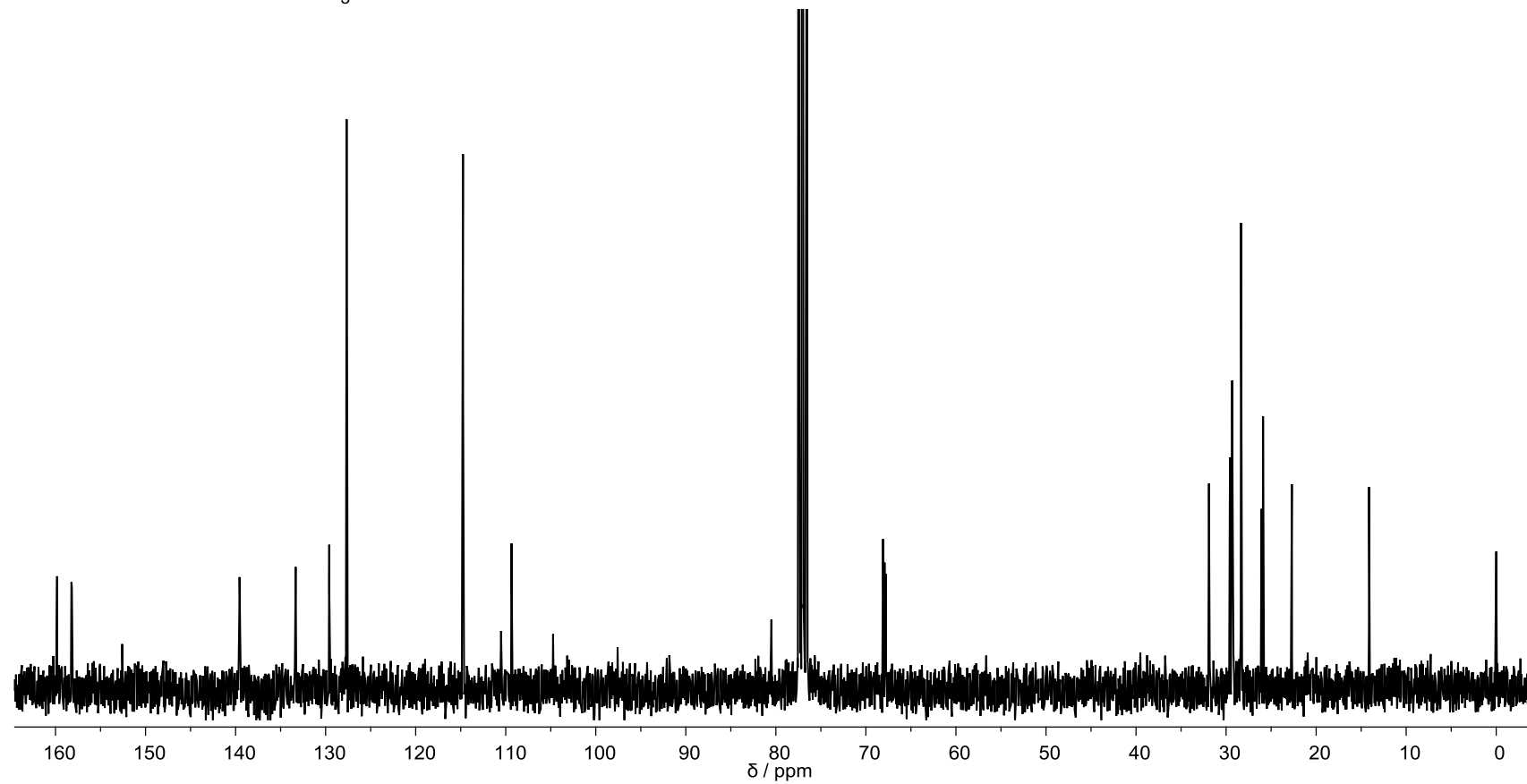
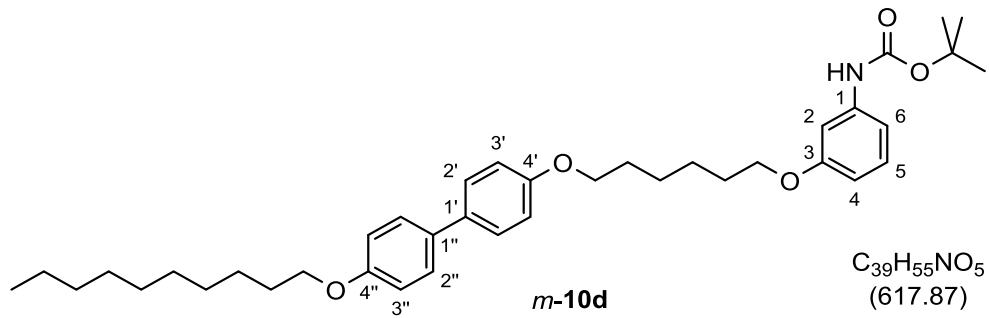
Acquisition Date 13.08.2013 12:17:37
 Operator wo/tri
 Instrument micrOTOF-Q 43

Acquisition Parameter

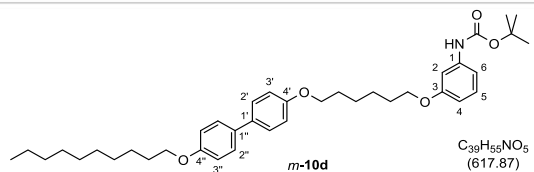
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Scan End	2500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste







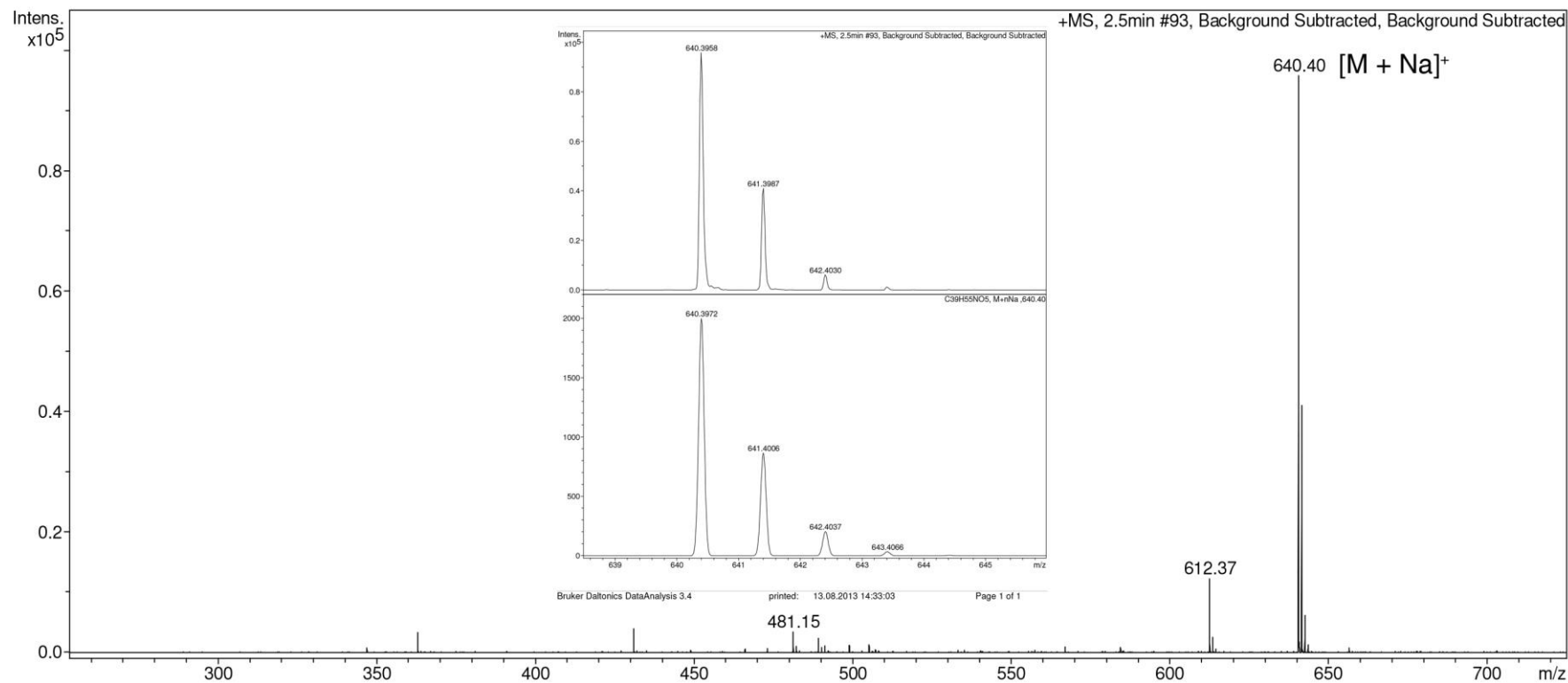
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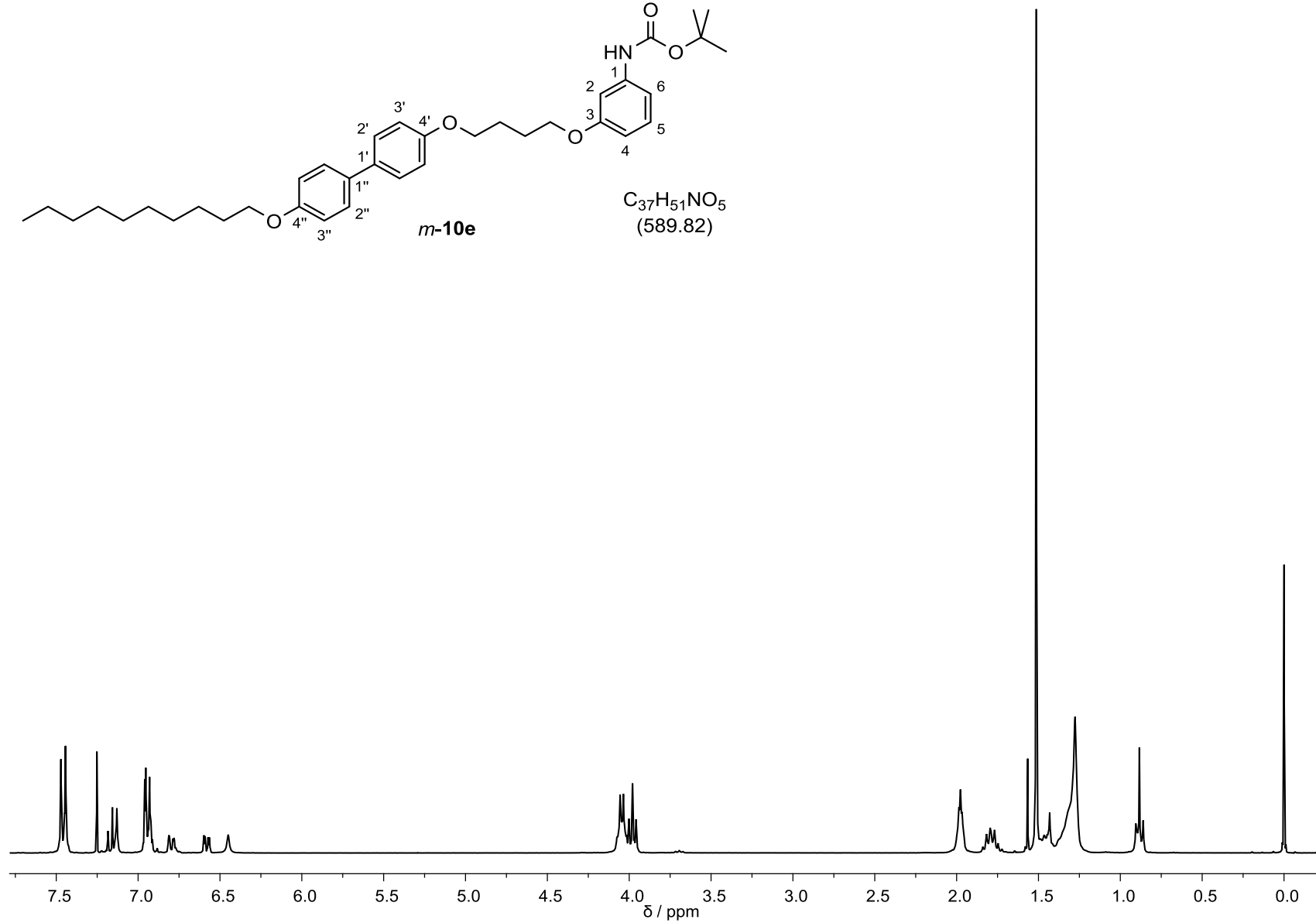
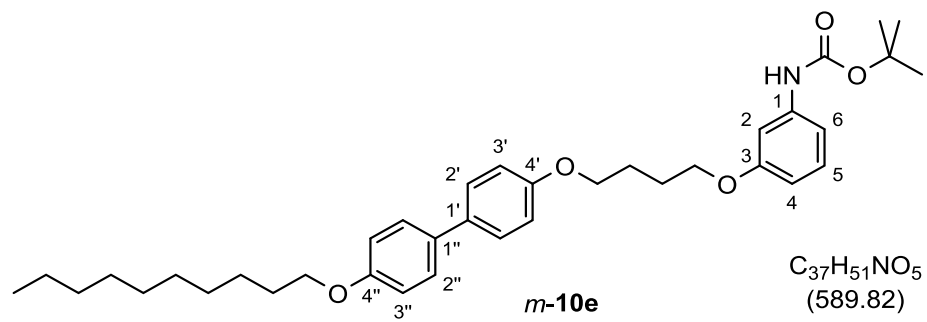


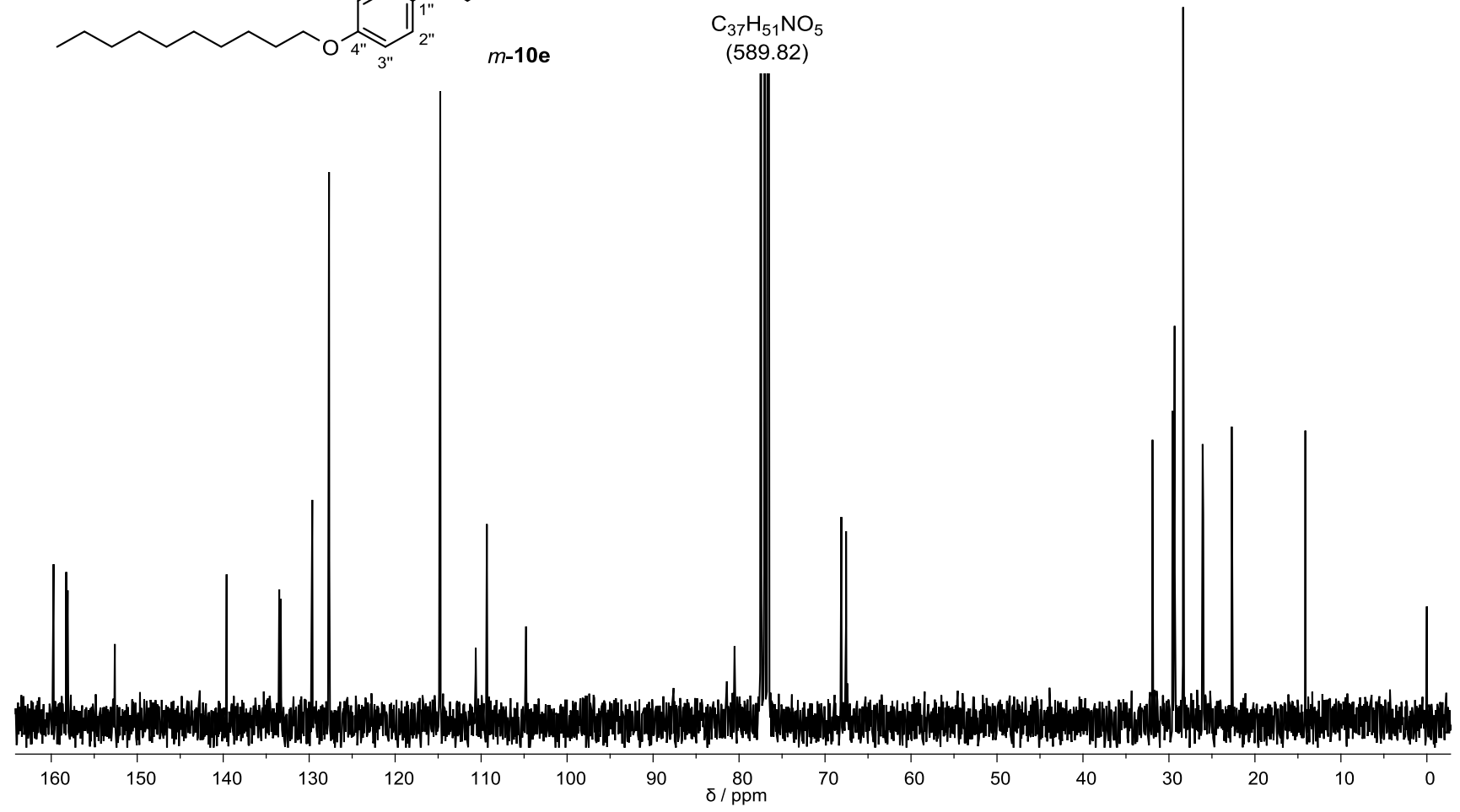
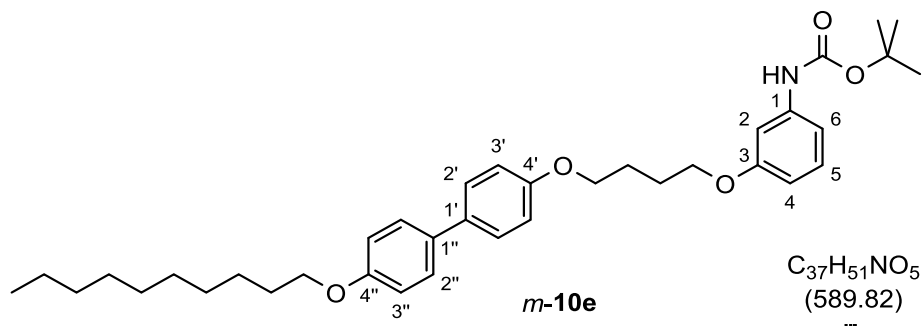
Acquisition Date 13.08.2013 12:11:28
 Operator wo/tri
 Instrument micrOTOF-Q 43

Acquisition Parameter

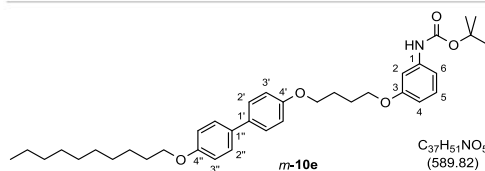
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Scan End	2500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste







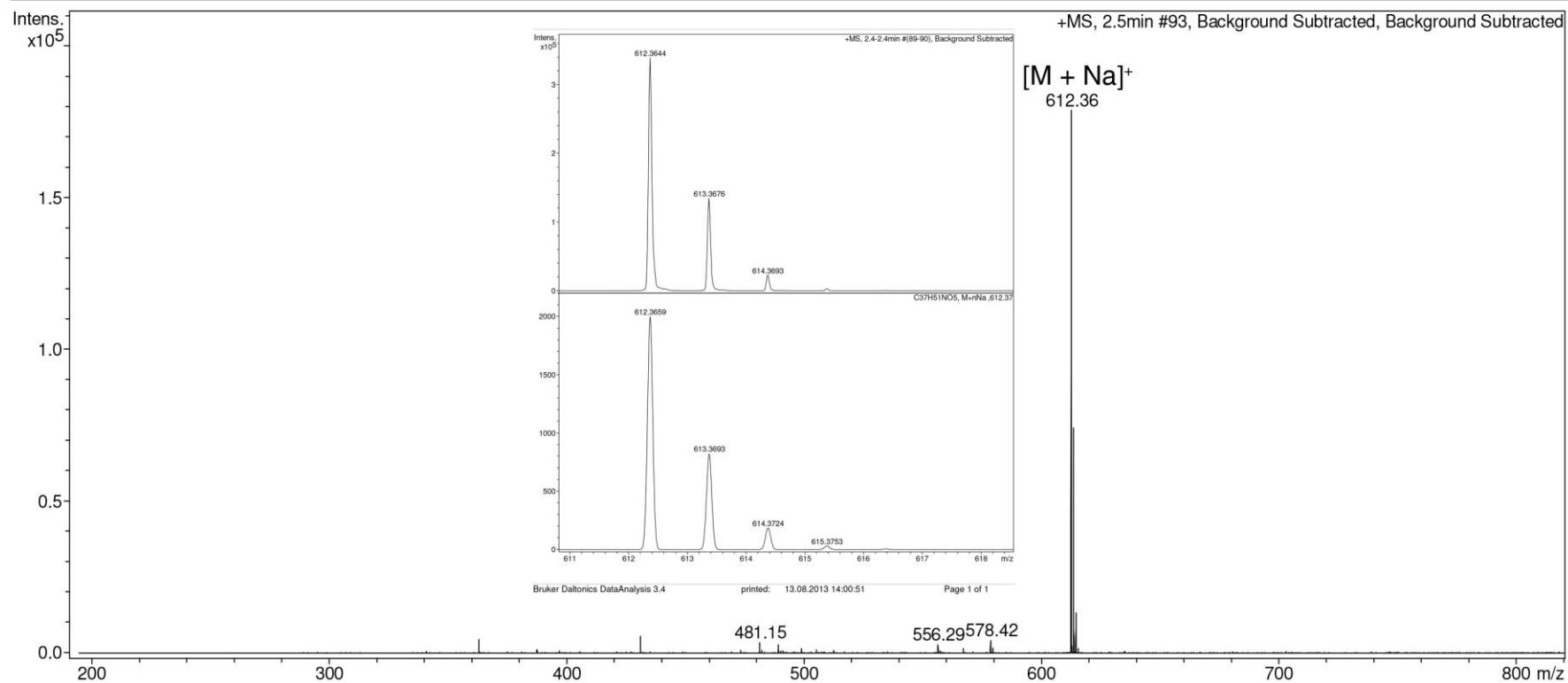
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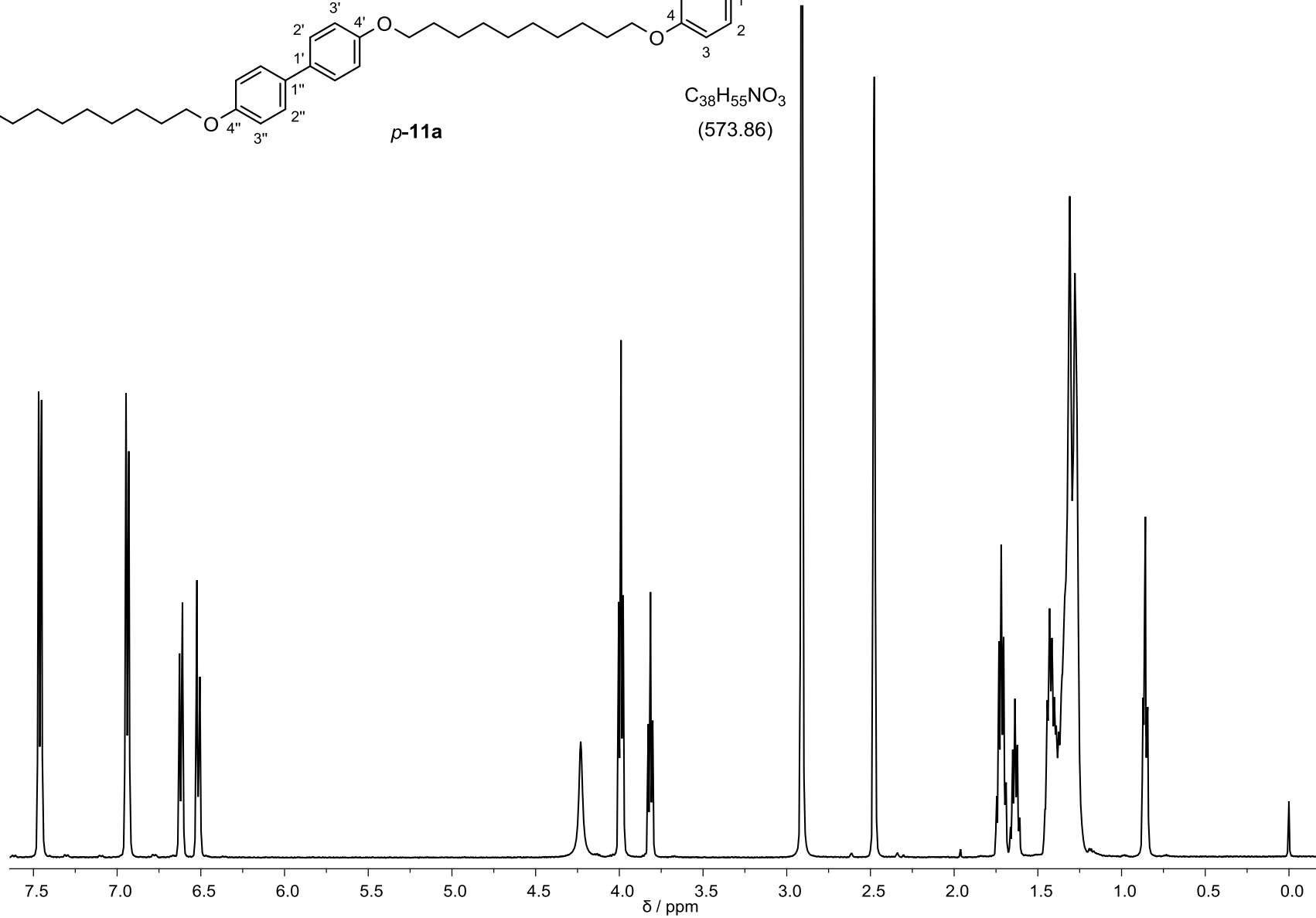
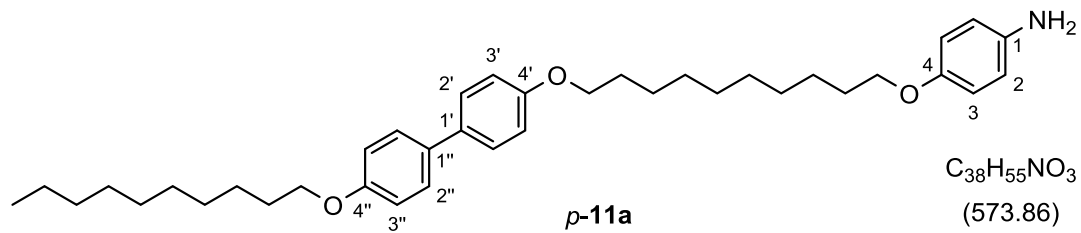


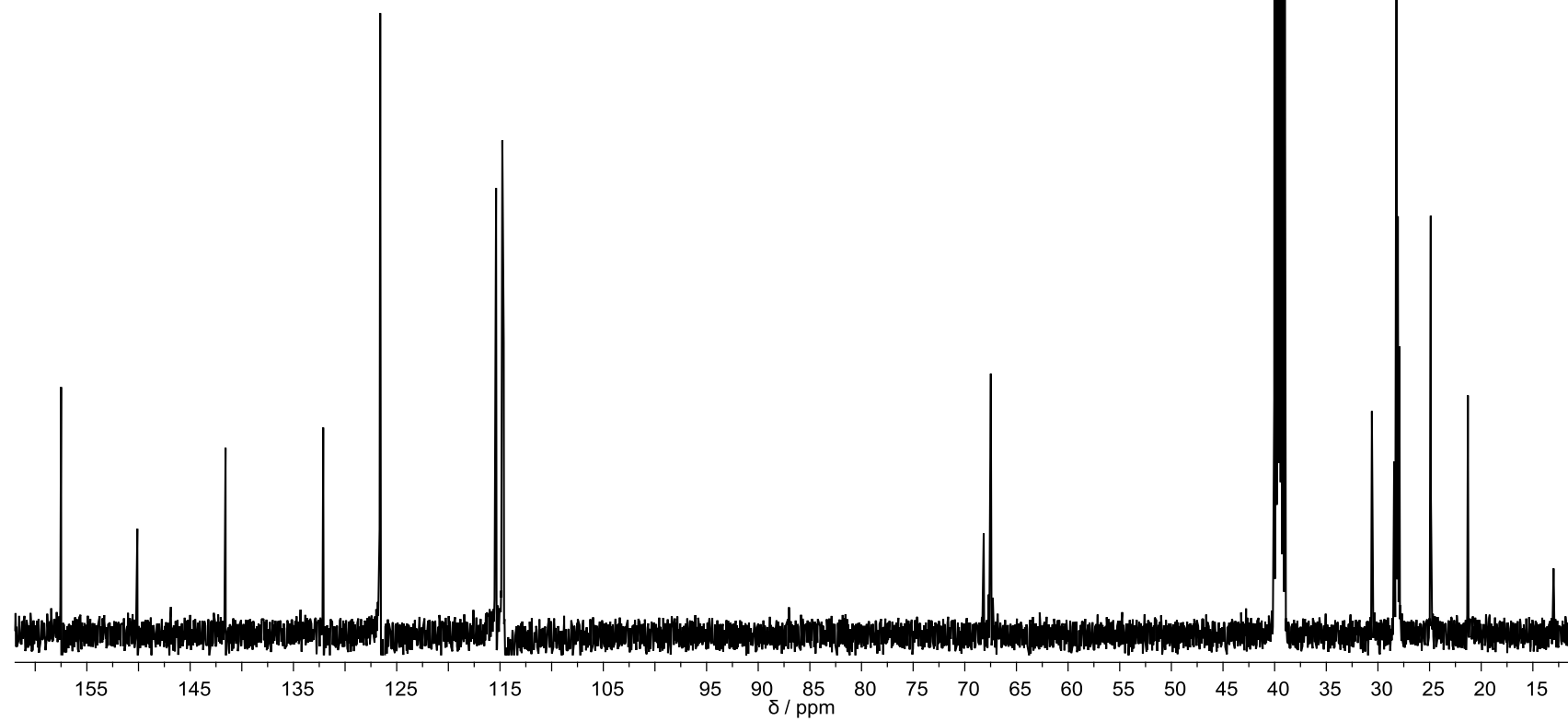
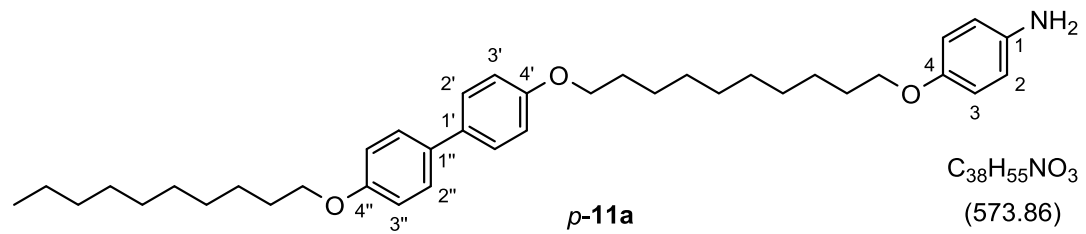
Acquisition Date 13.08.2013 12:05:22
 Operator wo/tri
 Instrument micrOTOF-Q 43

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
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Scan End	2500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste







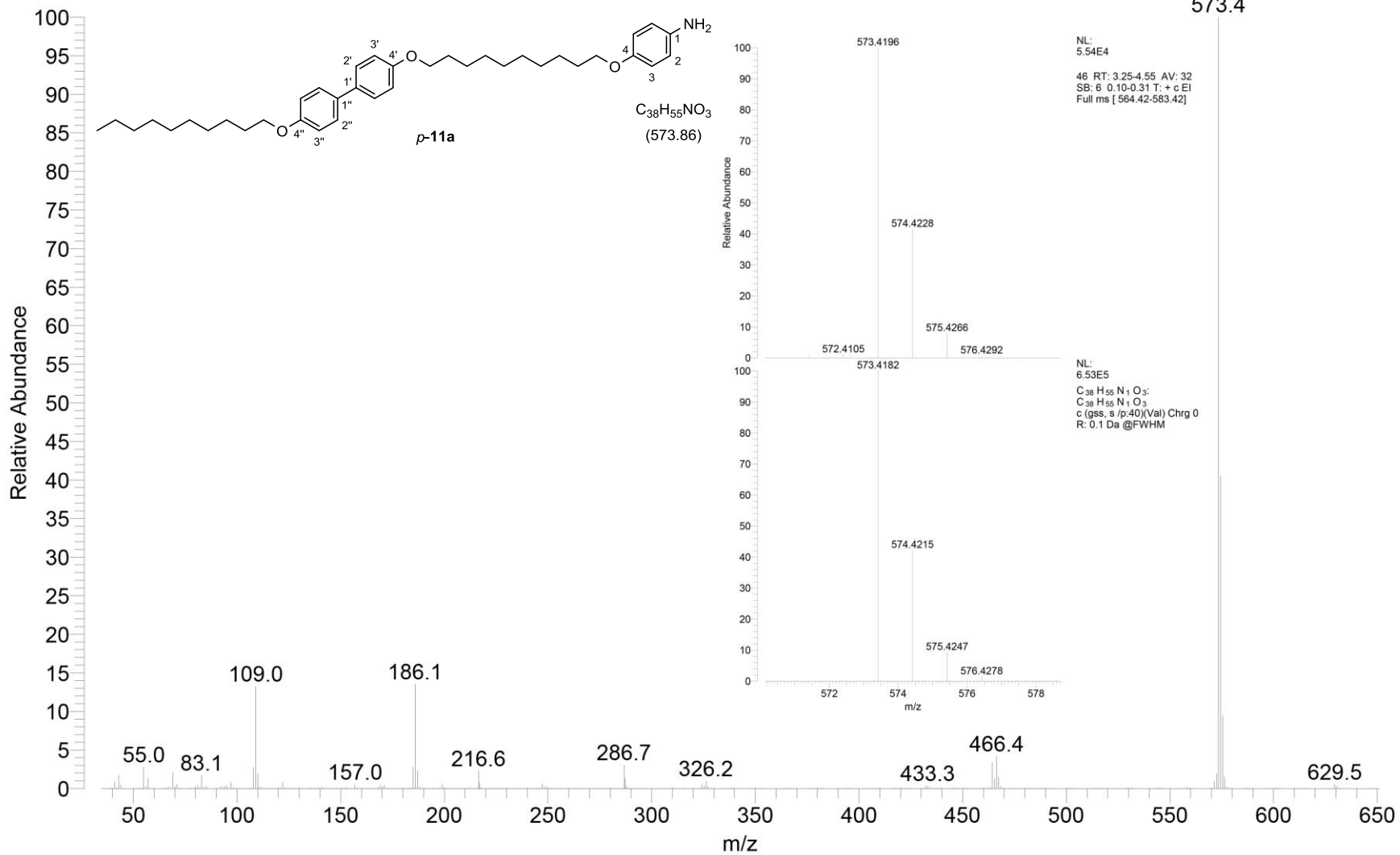
El positiv-Ion, 70eV

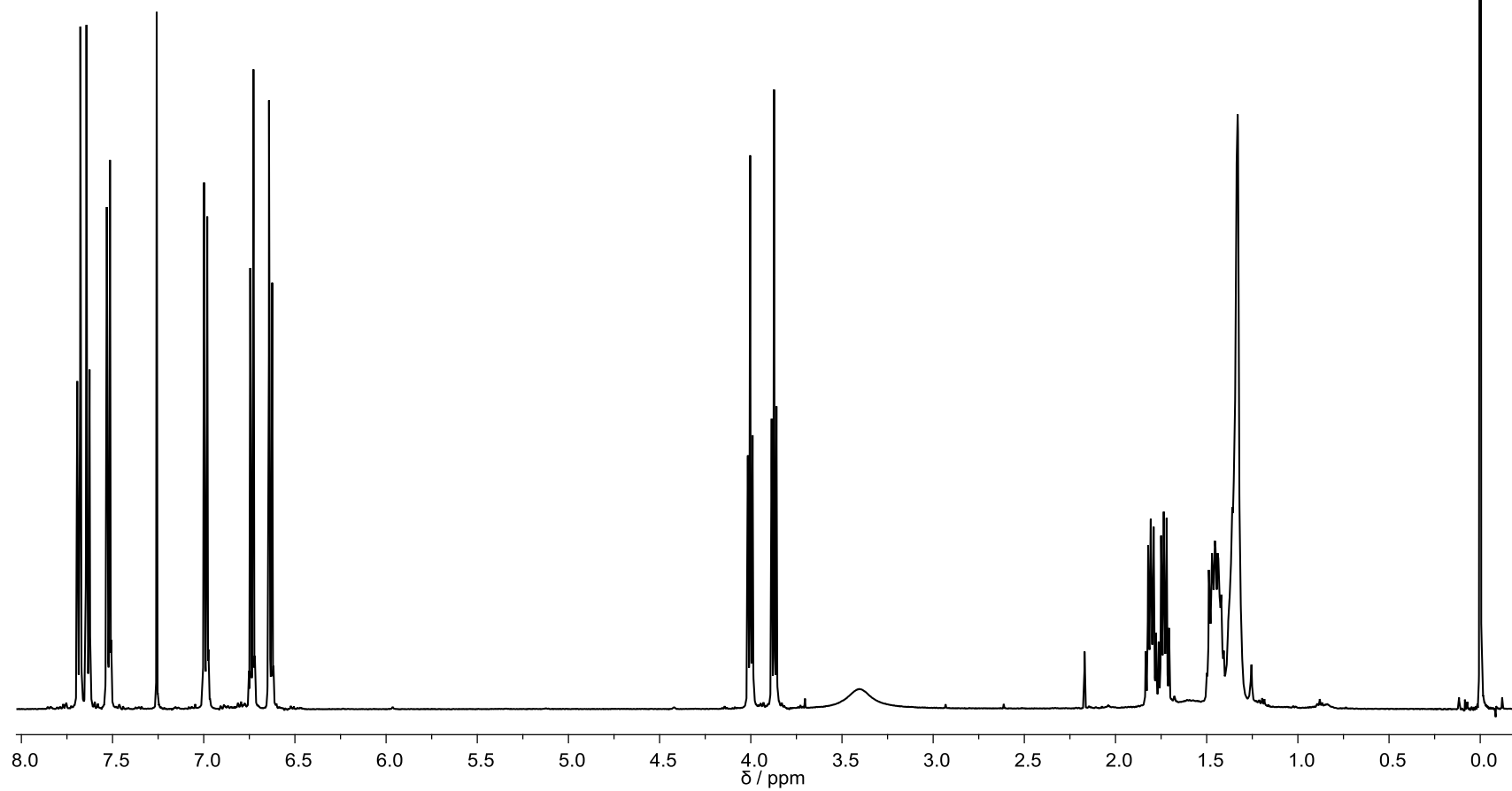
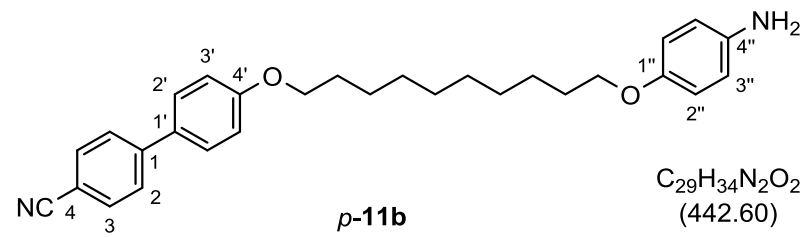
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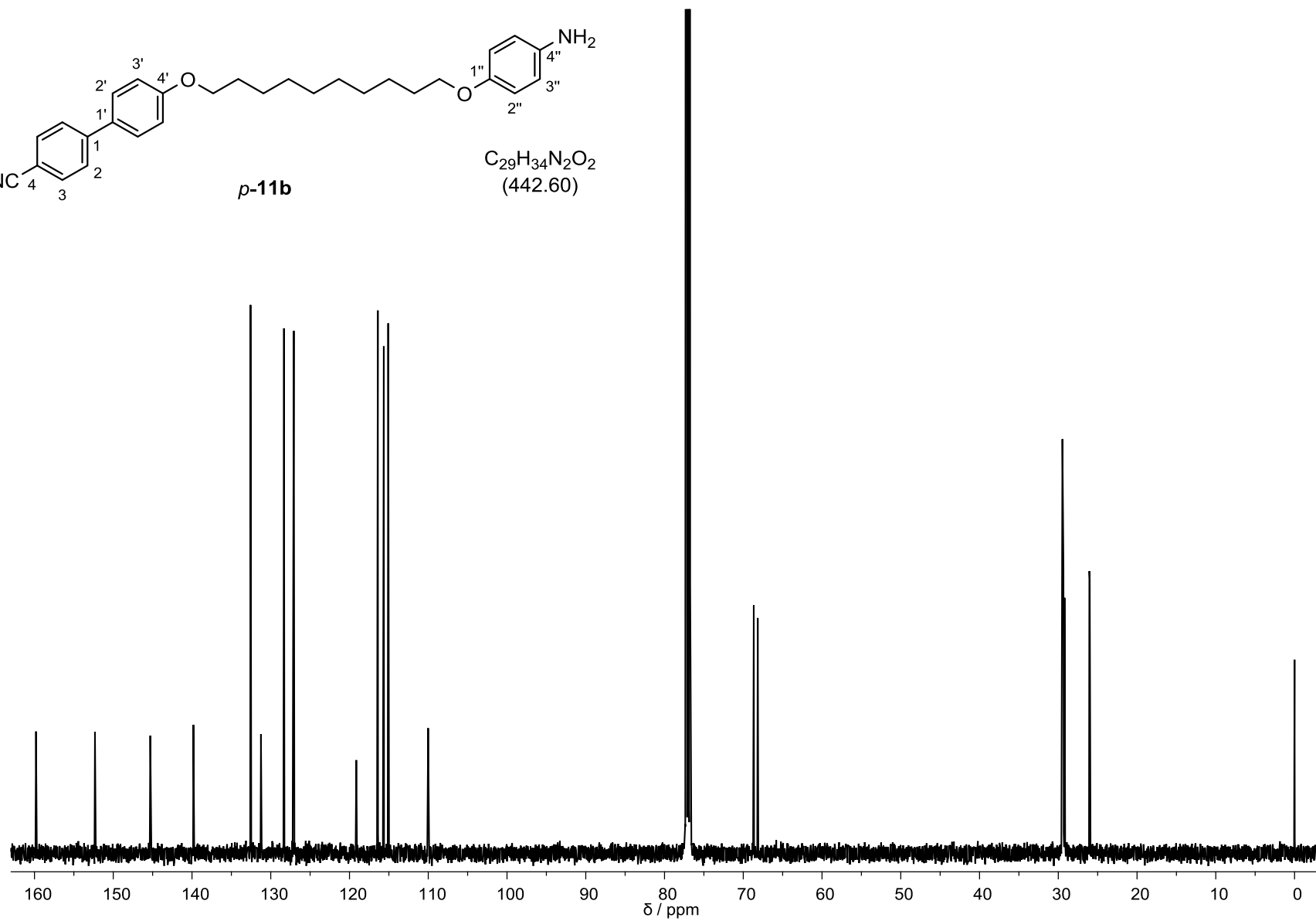
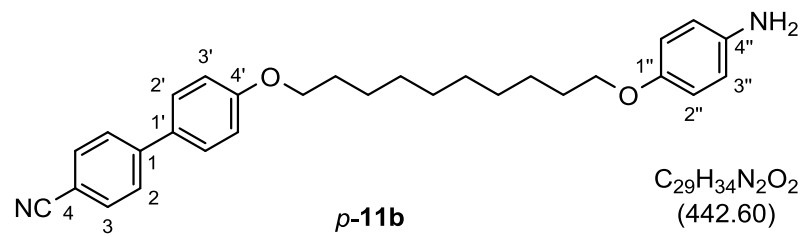
T: + c EI Full ms [34.50-850.50]

Tquelle=190°C
Tprobe=260°C

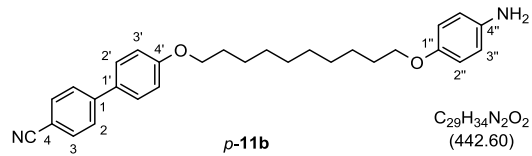
8/5/2013 8:29:00 AM
C38H55NO3







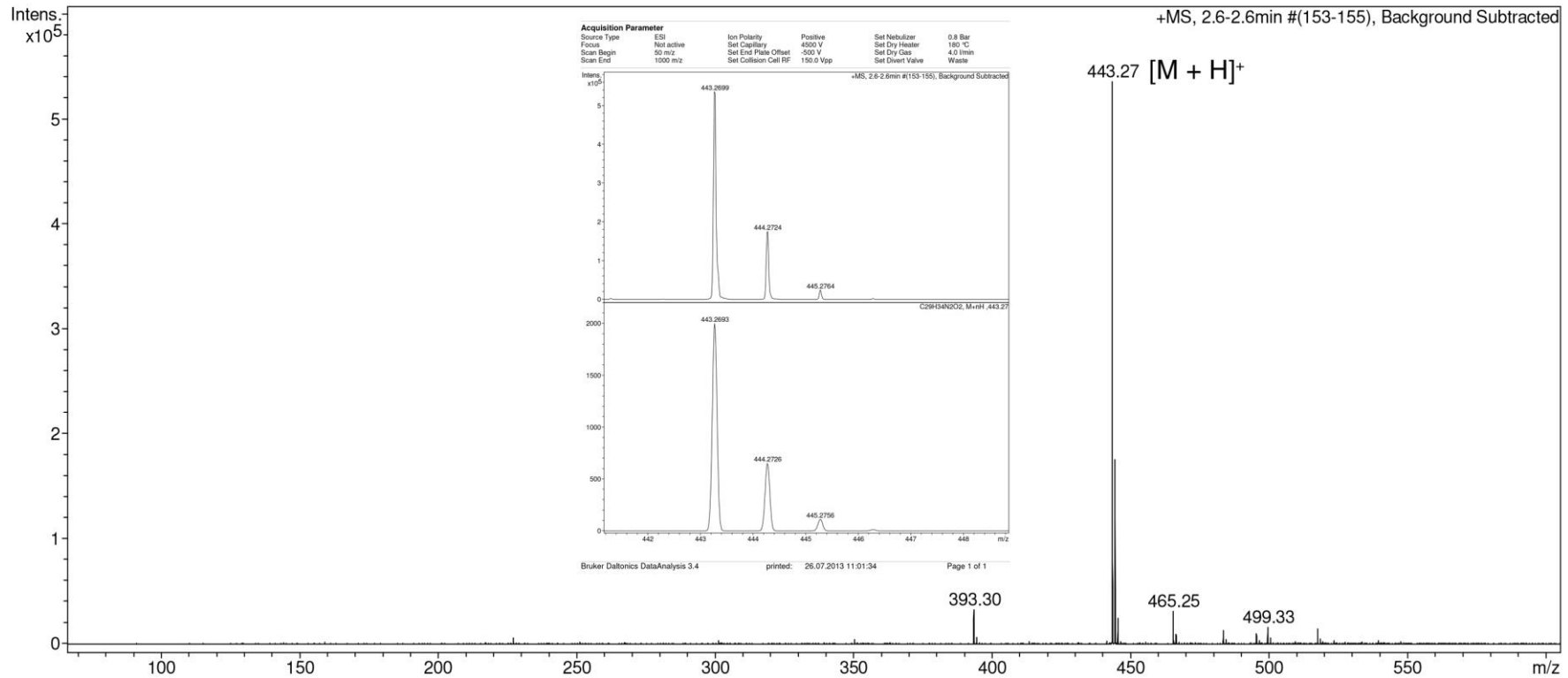
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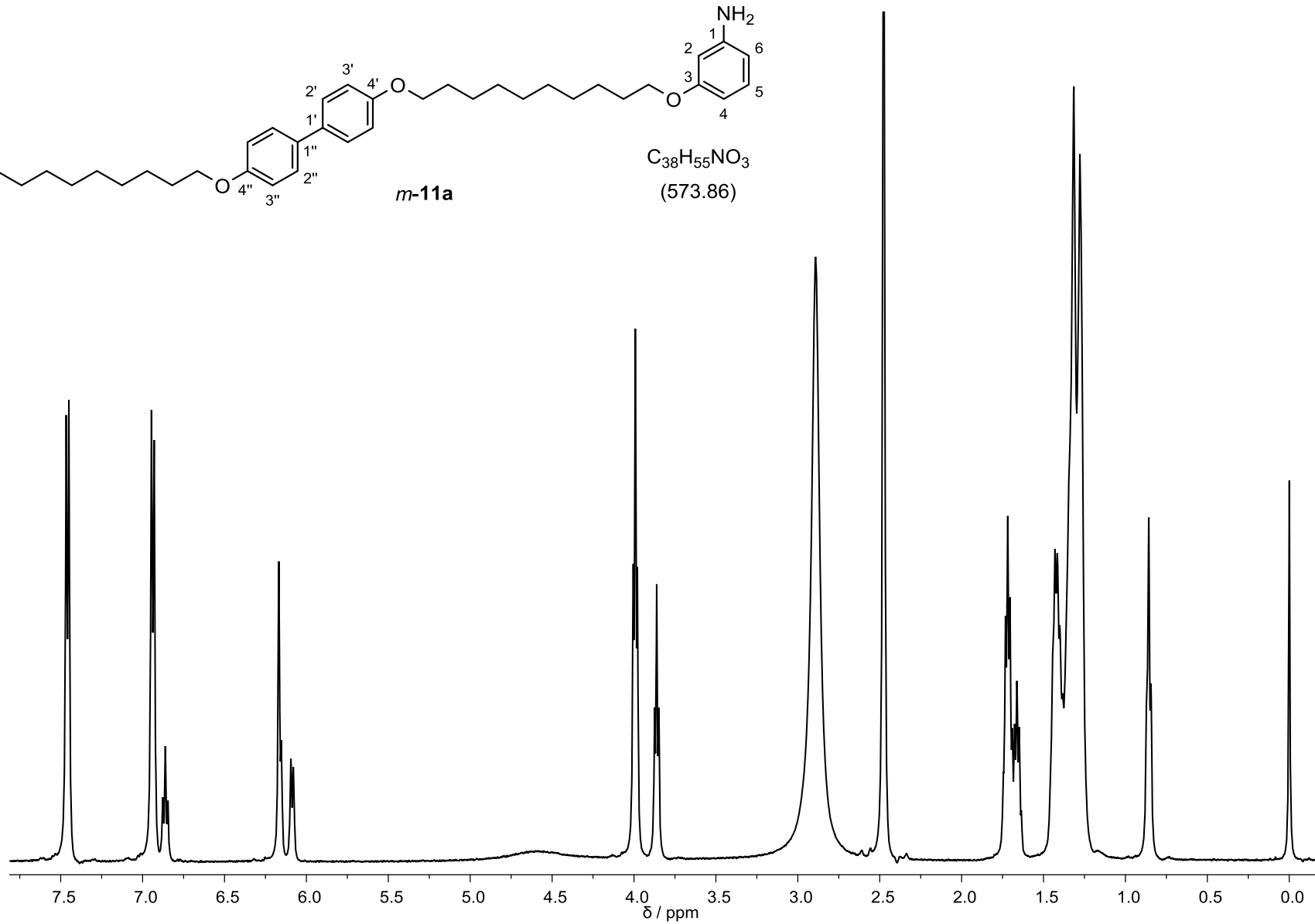
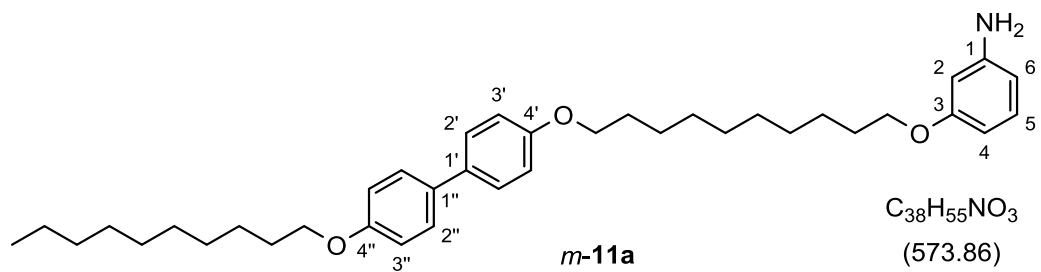


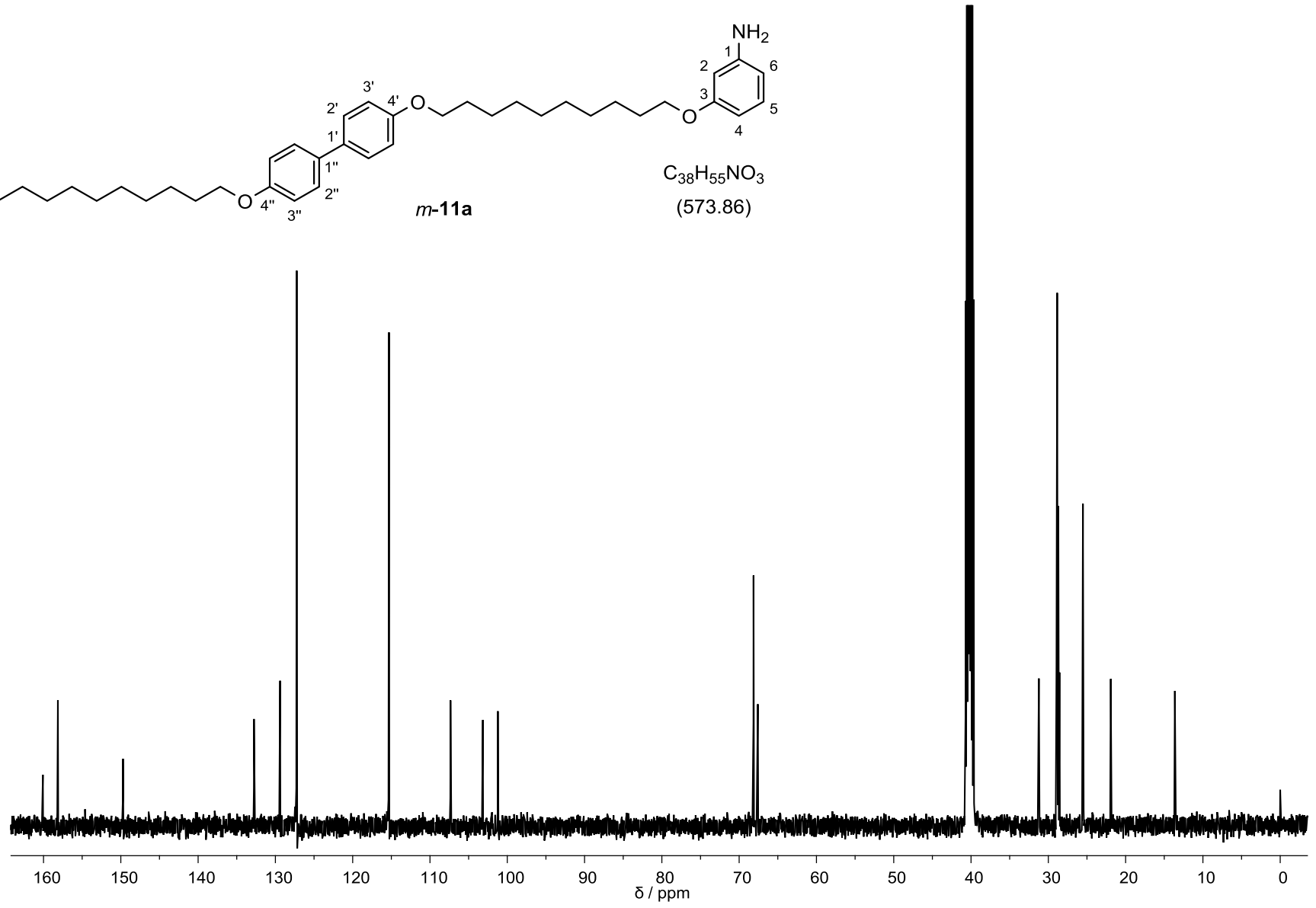
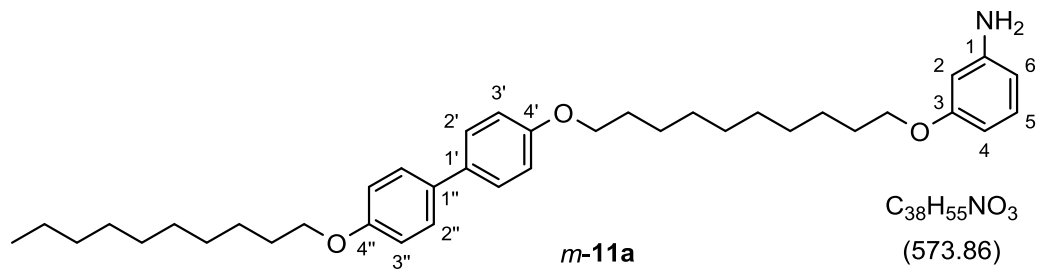
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Operator wo/tri
Instrument micrOTOF-Q 43

Acquisition Parameter

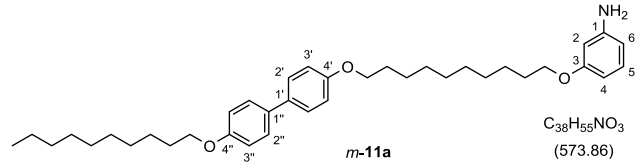
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Scan End	1000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste







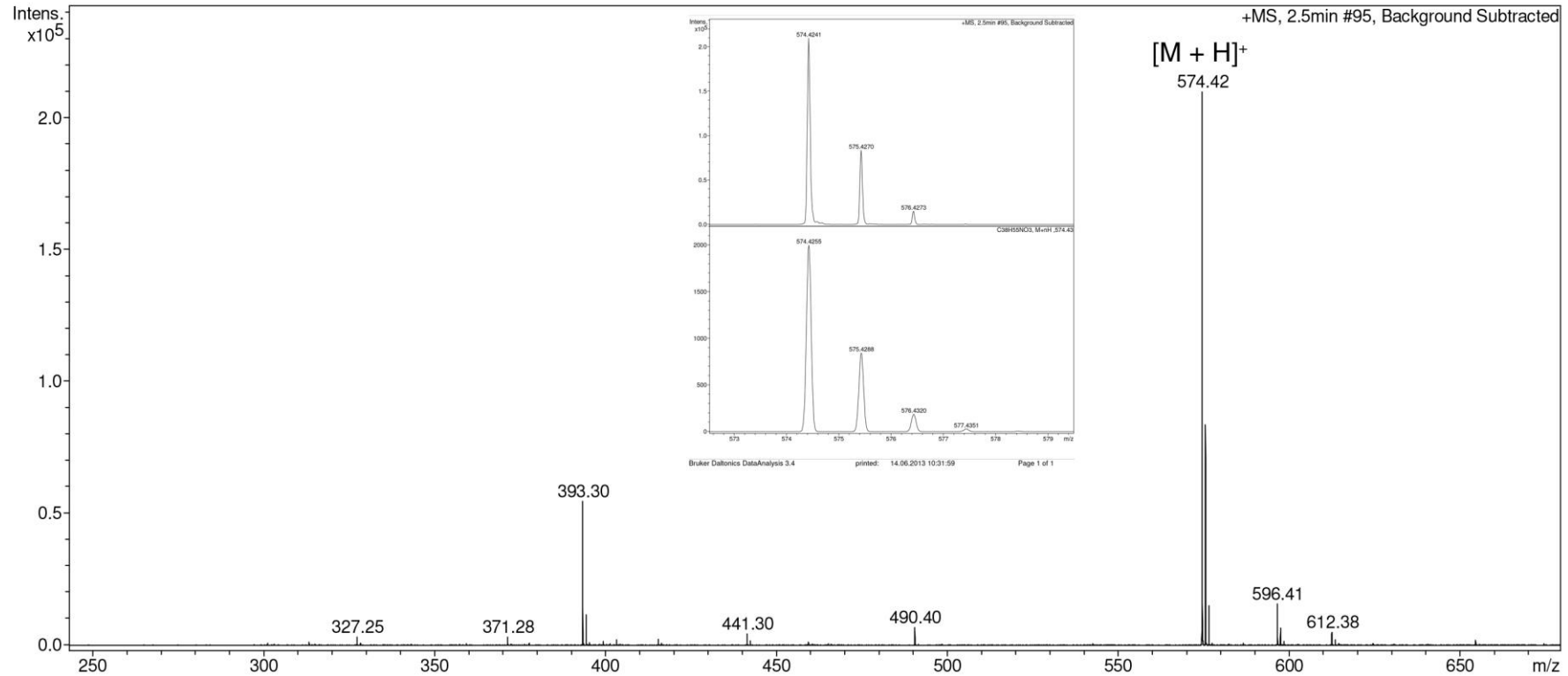
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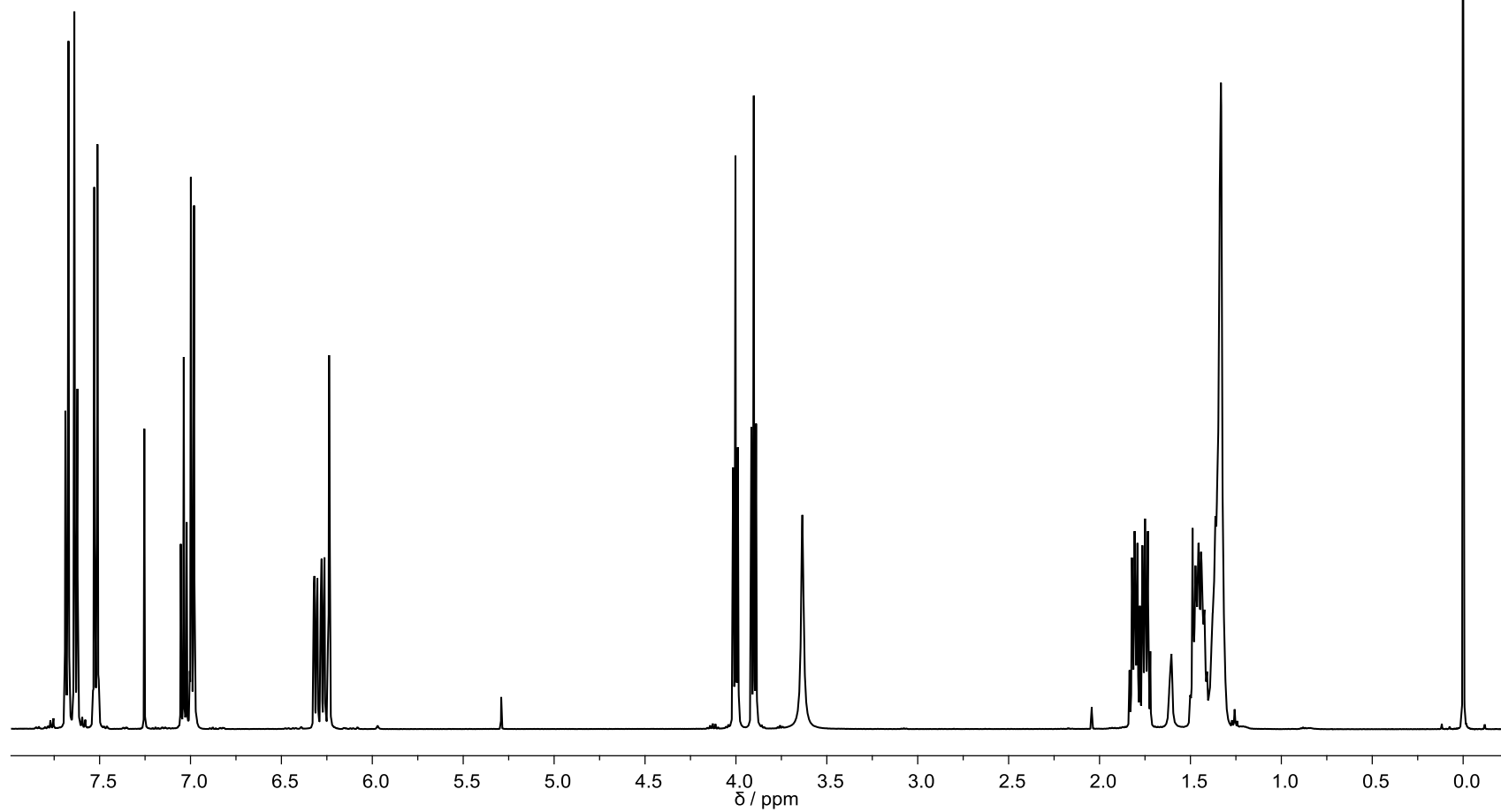
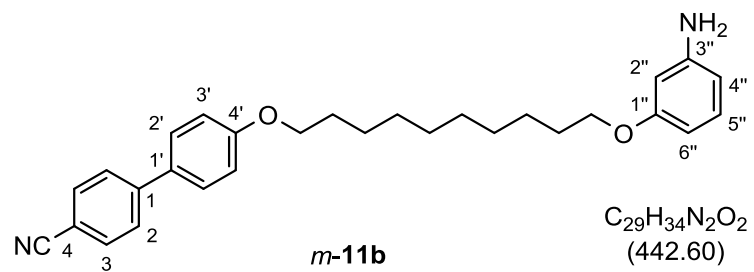


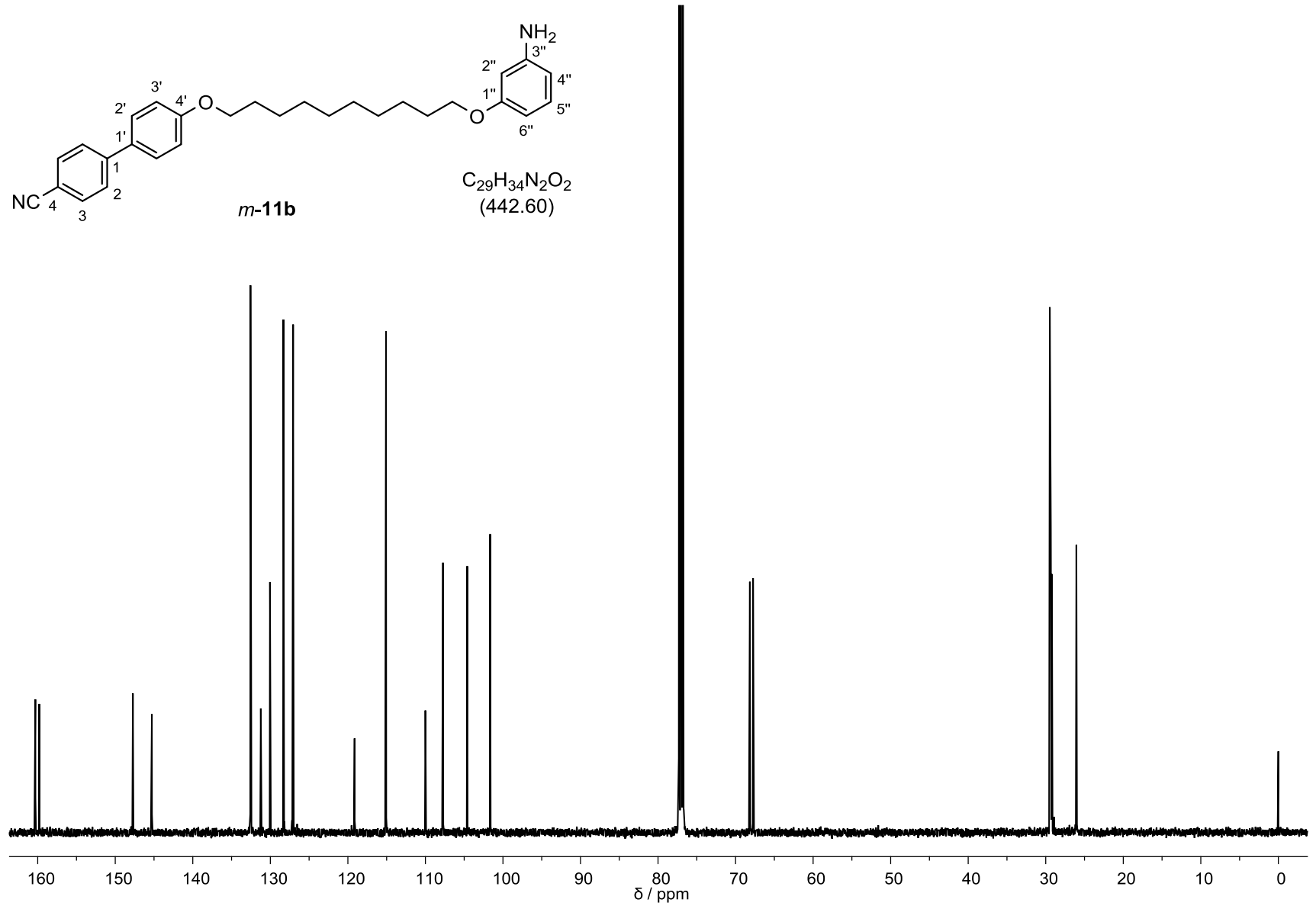
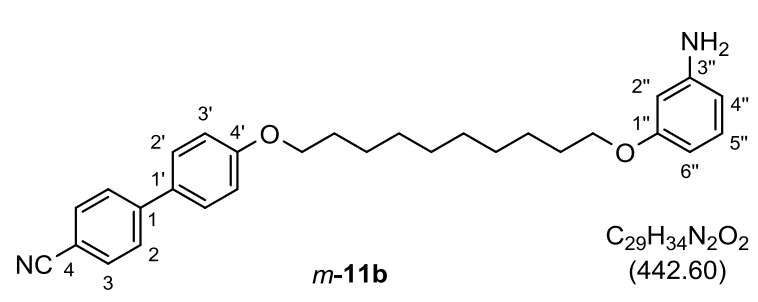
Acquisition Date 14.06.2013 09:28:05
 Operator wo/tri
 Instrument micrOTOF-Q 43

Acquisition Parameter

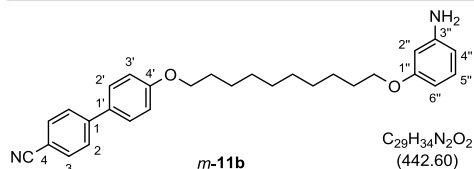
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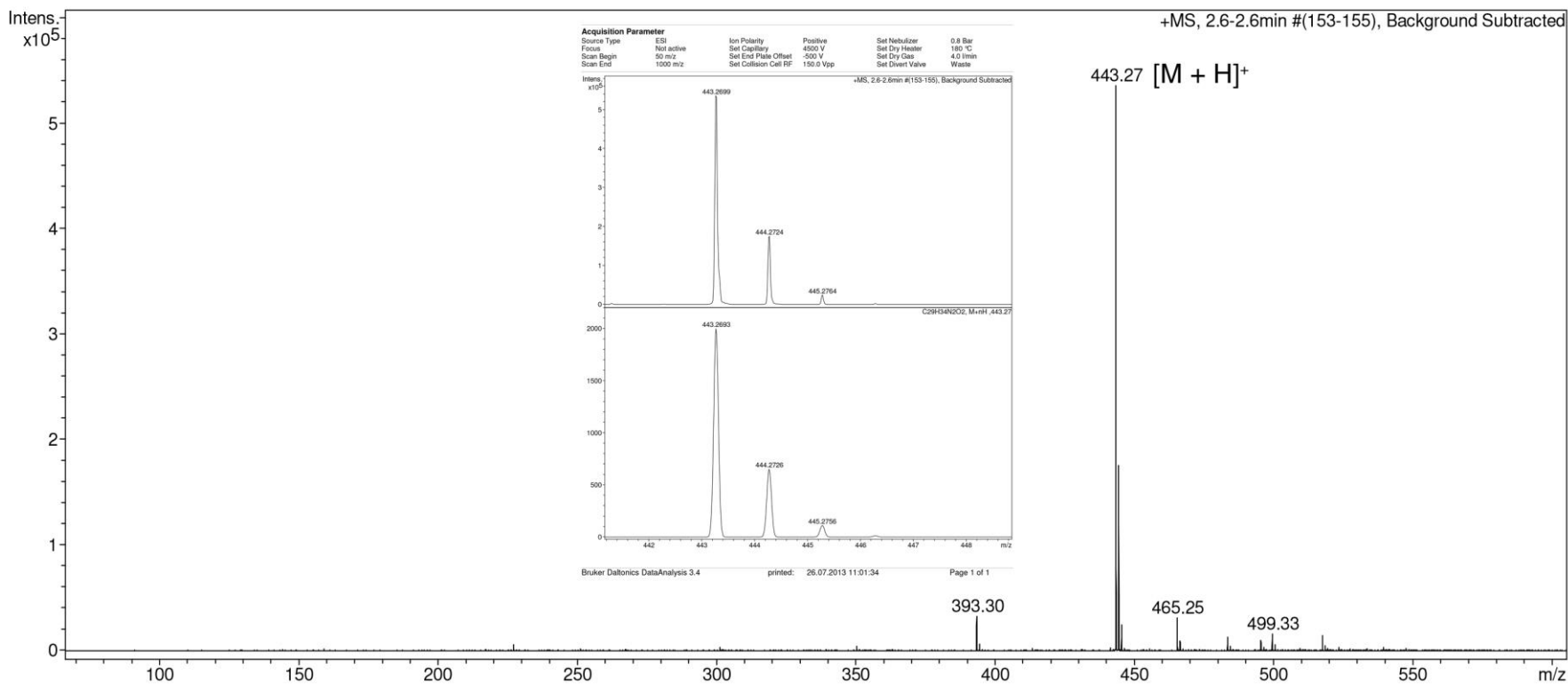
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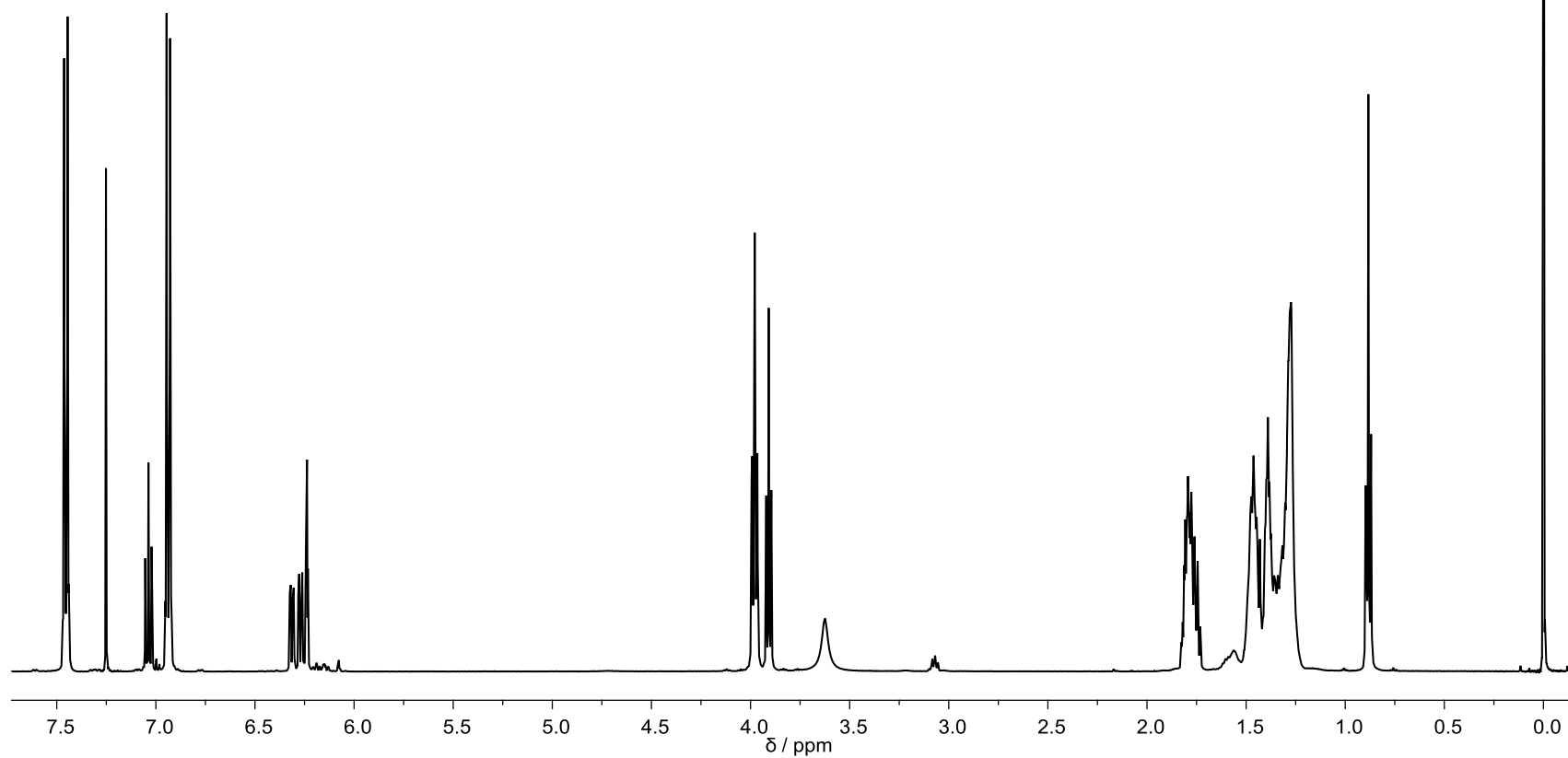
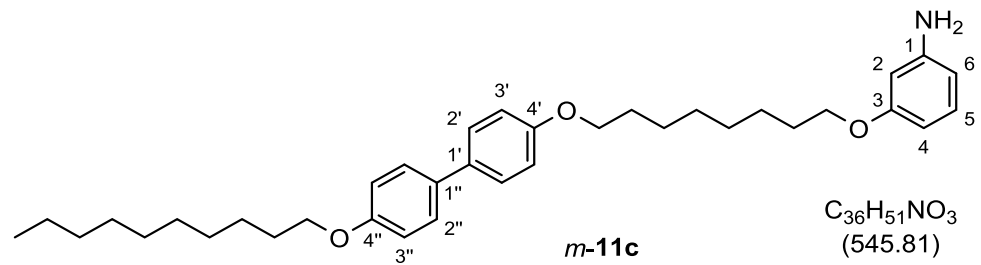


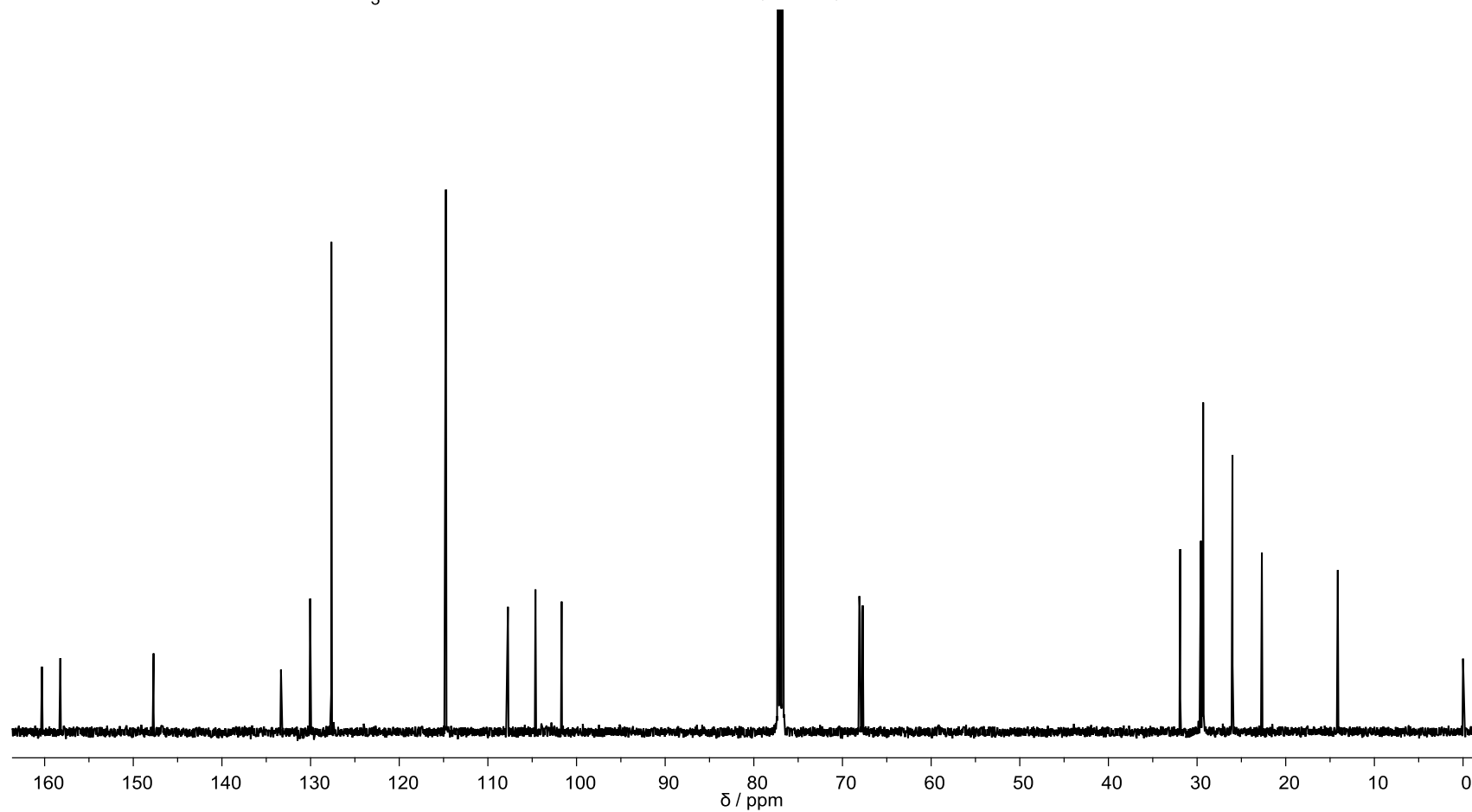
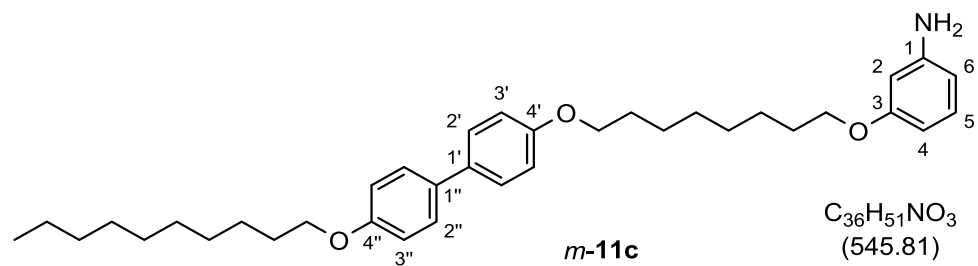
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 Operator wo/tri
 Instrument micrOTOF-Q 43

Acquisition Parameter

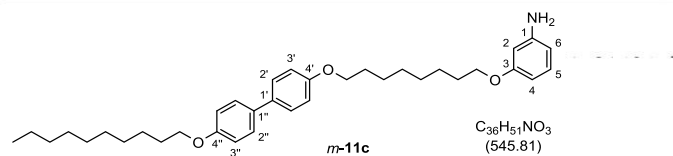
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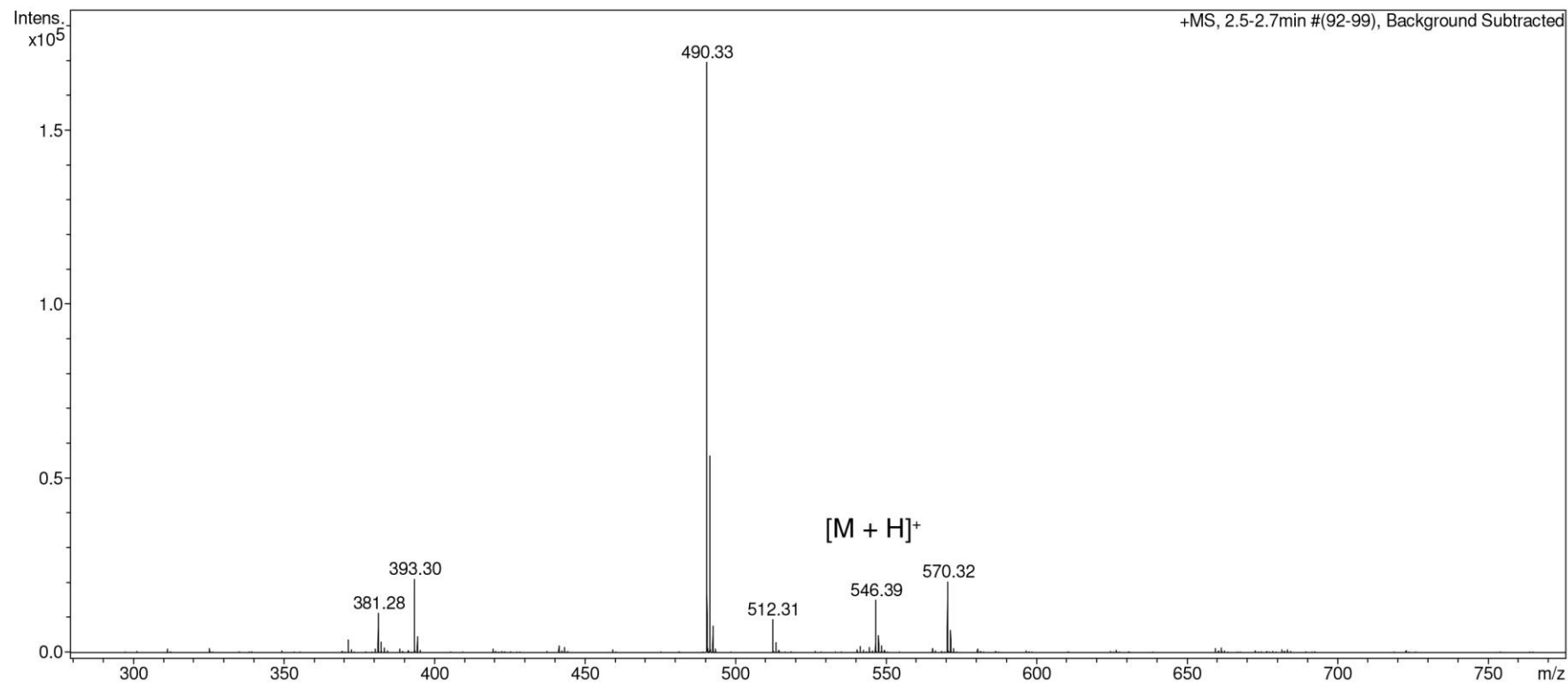
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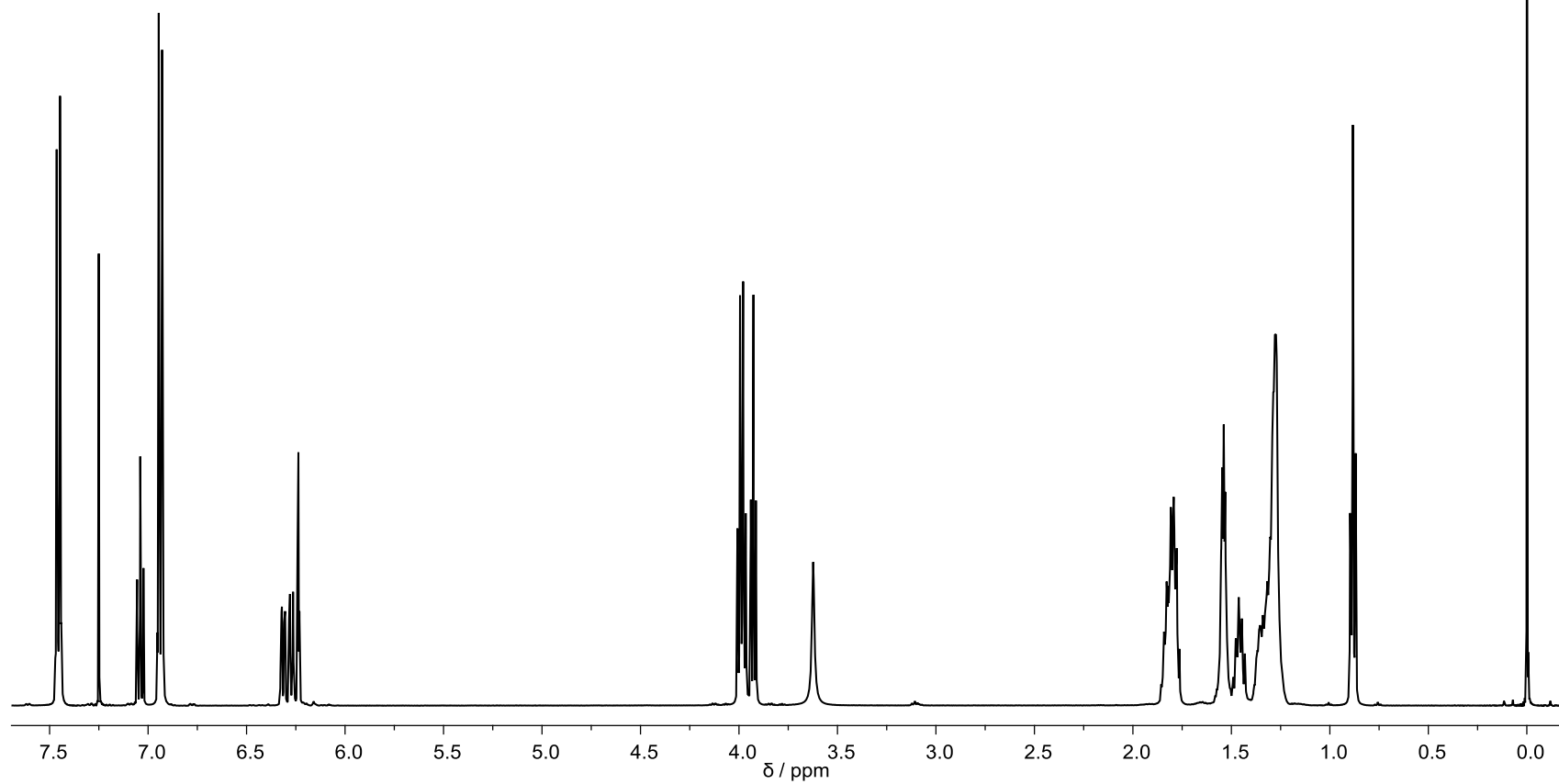
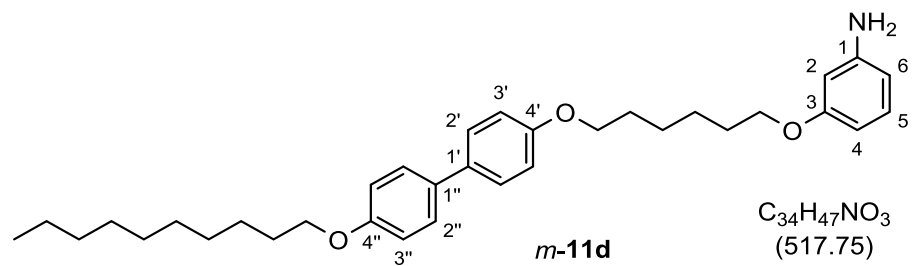


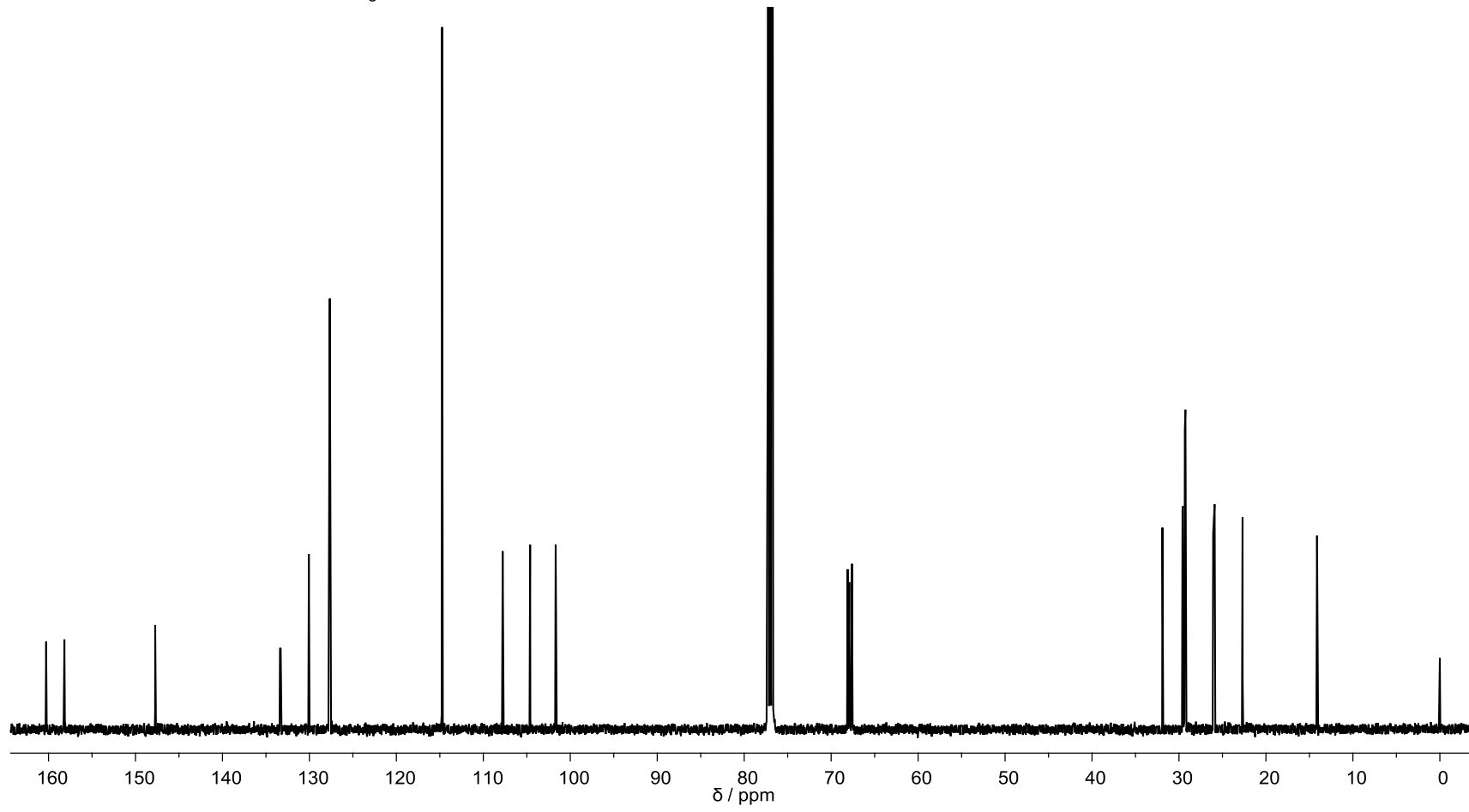
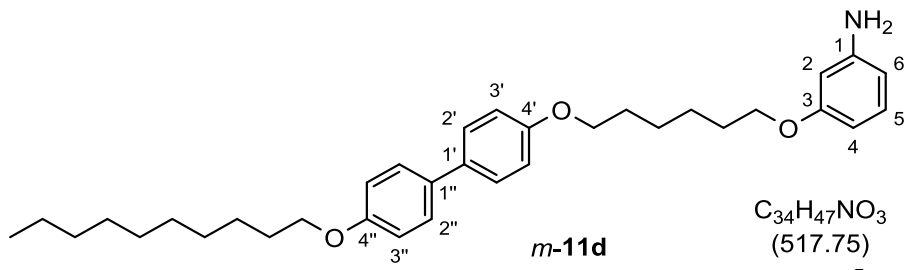
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Operator wo/tri
Instrument micrOTOF-Q 43

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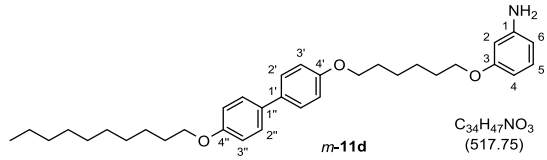
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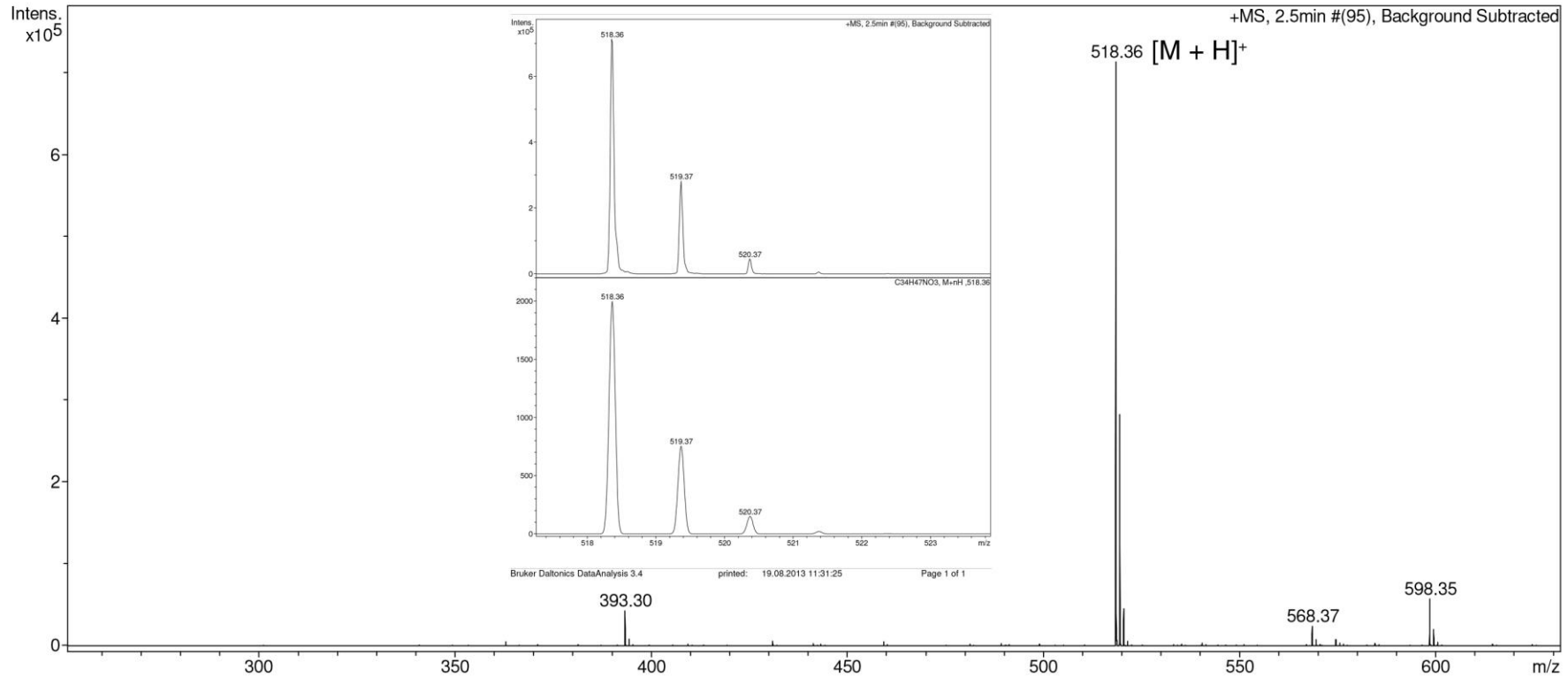
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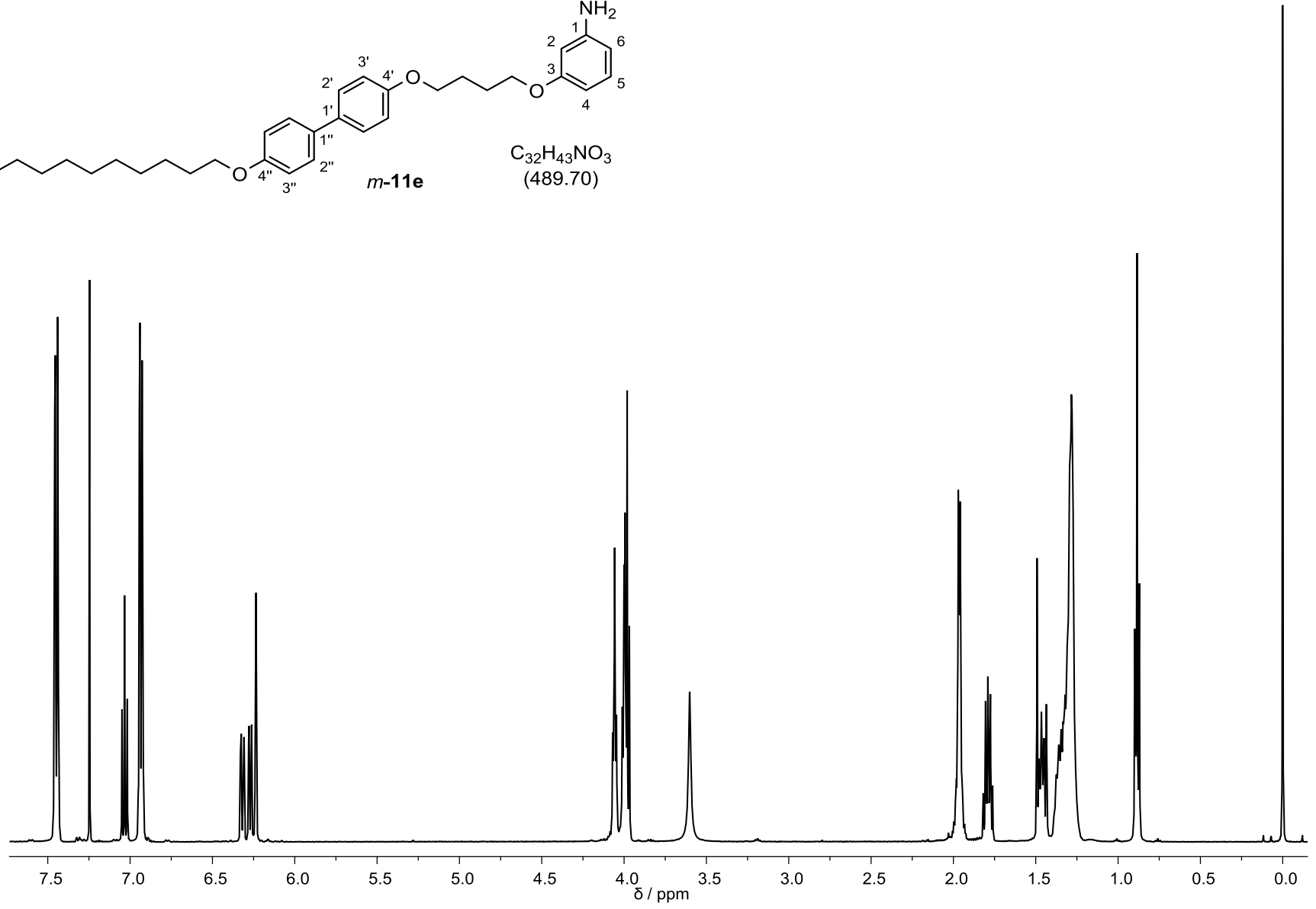
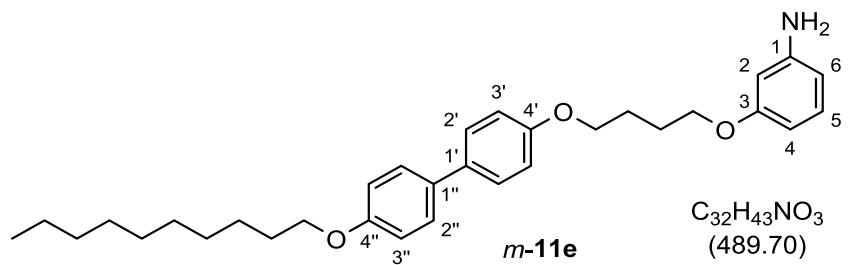


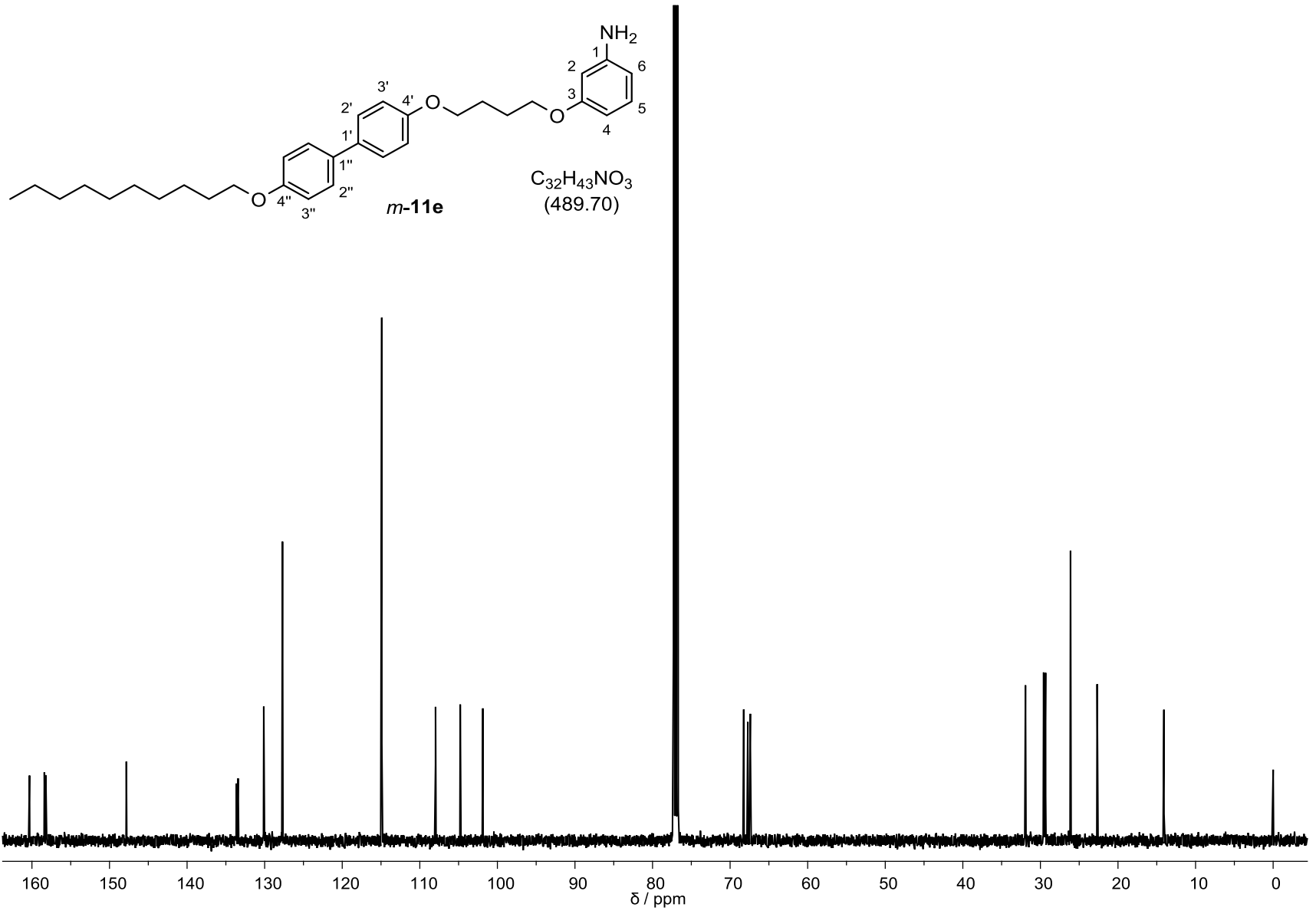
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 Operator wo/tri
 Instrument micrOTOF-Q 43

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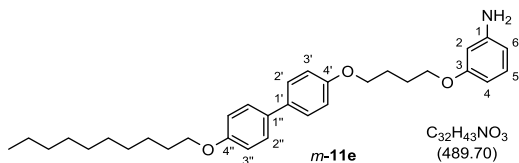
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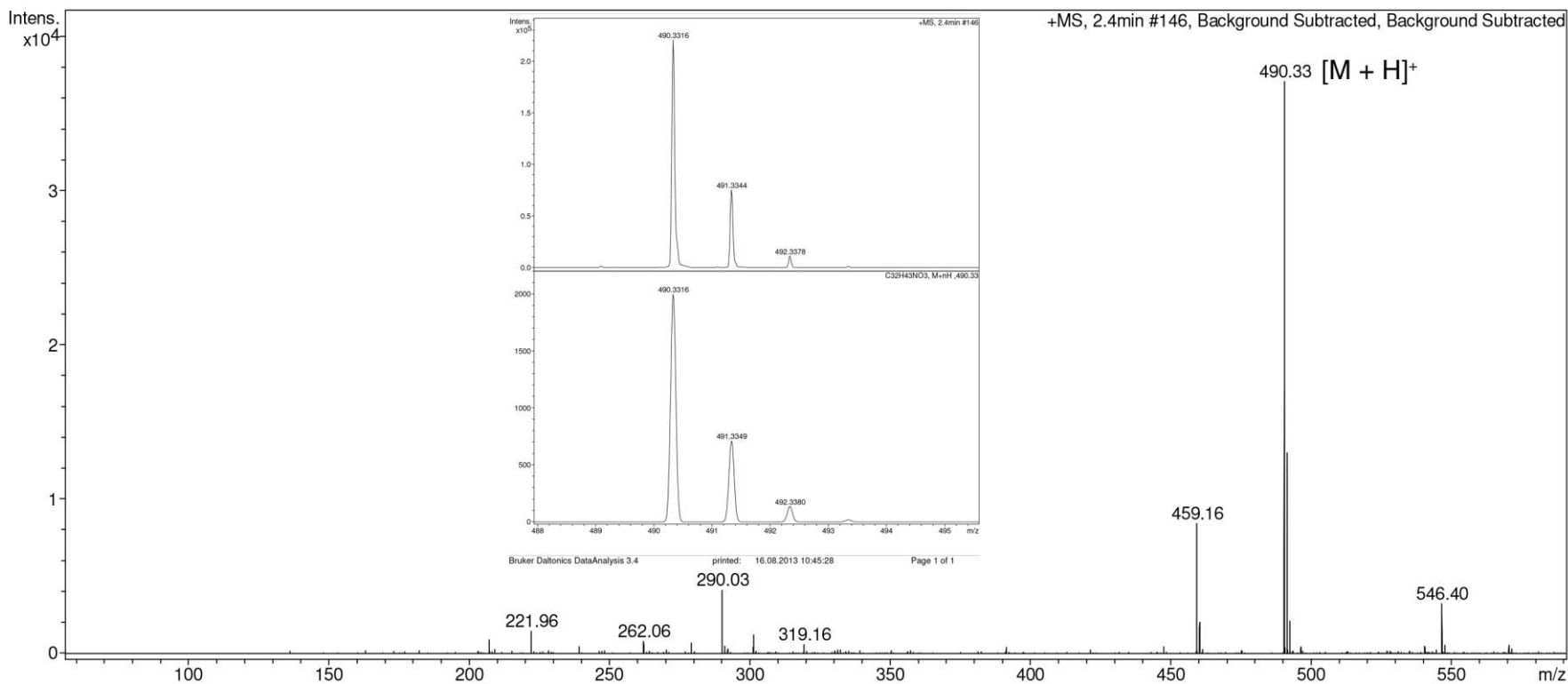
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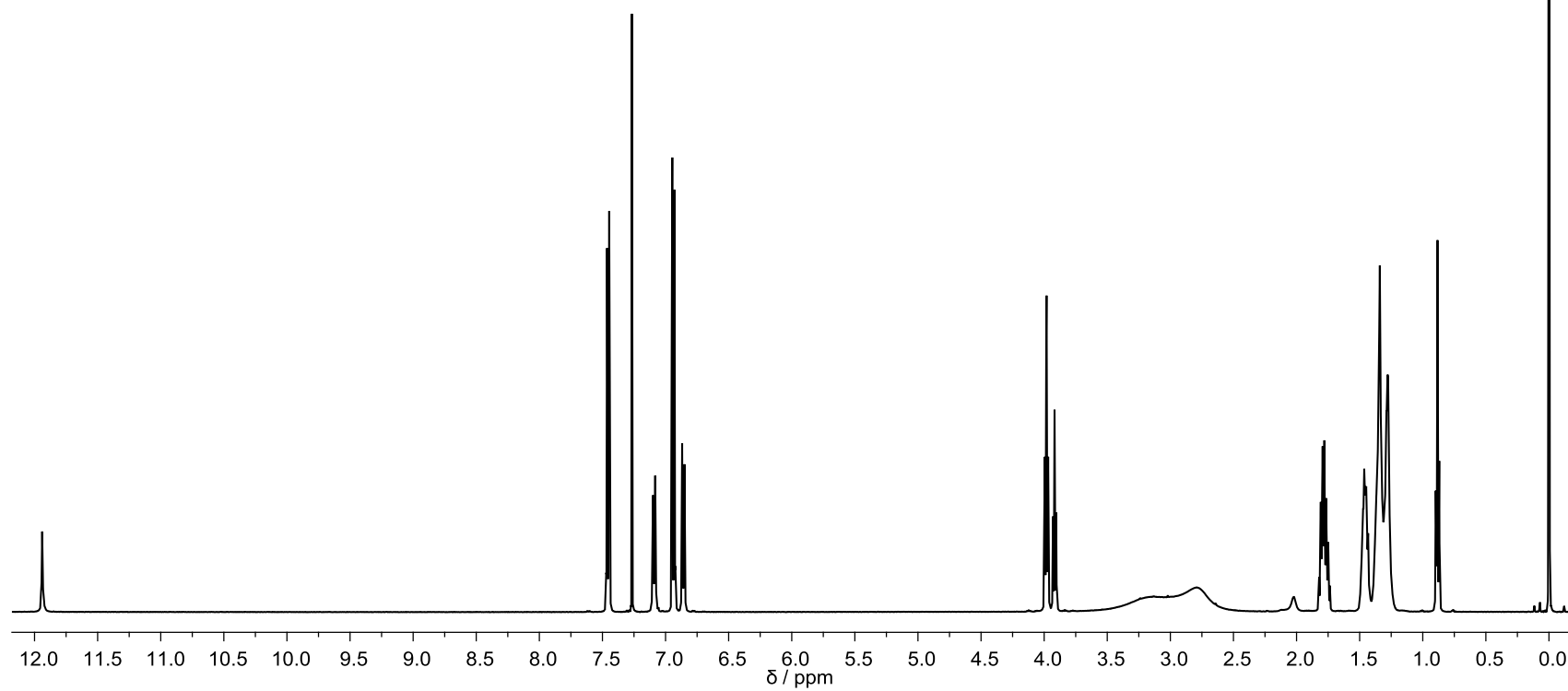
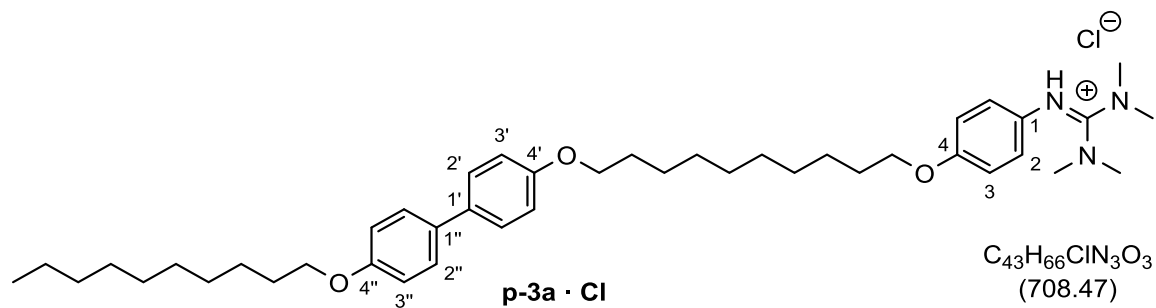


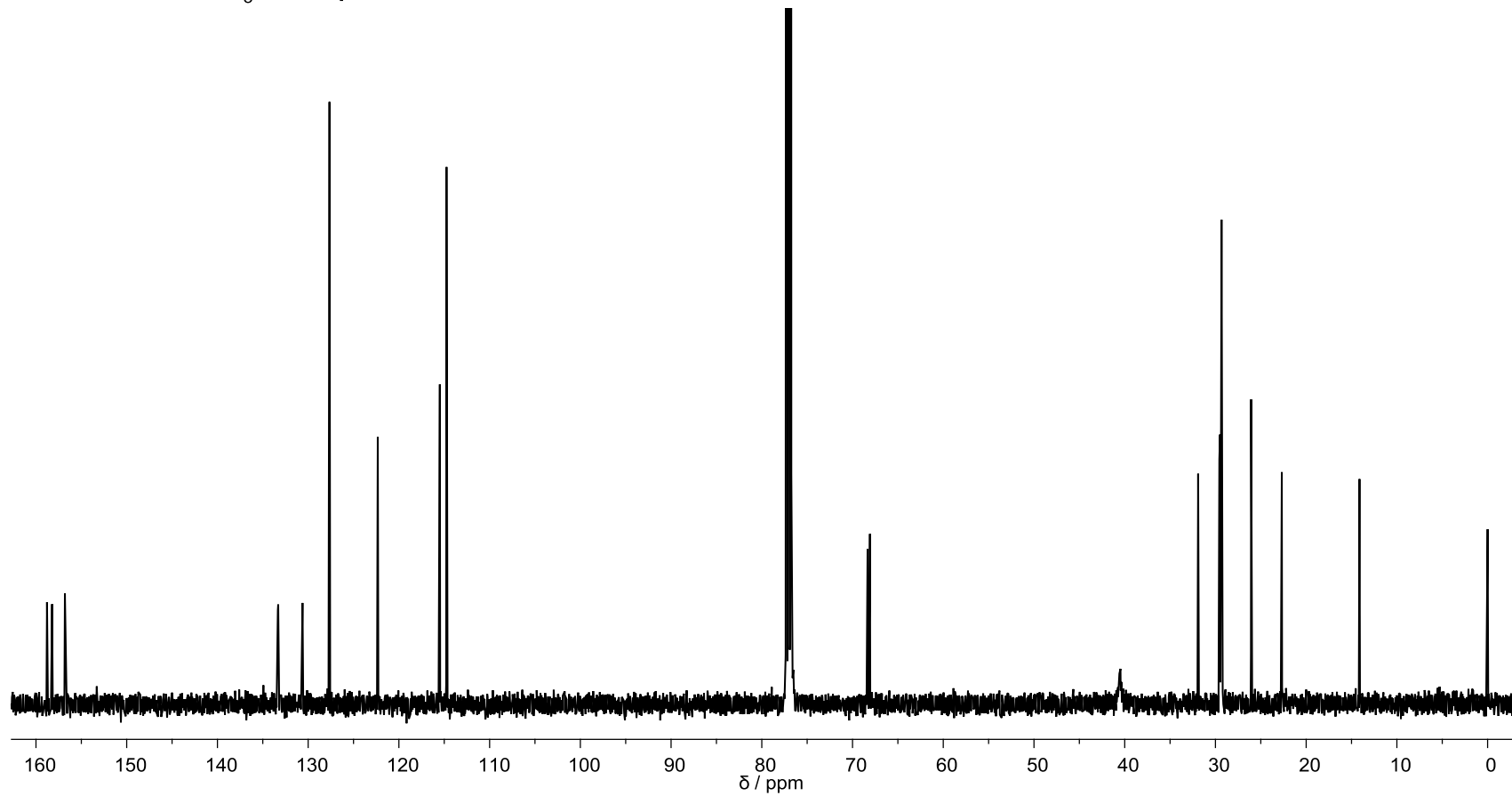
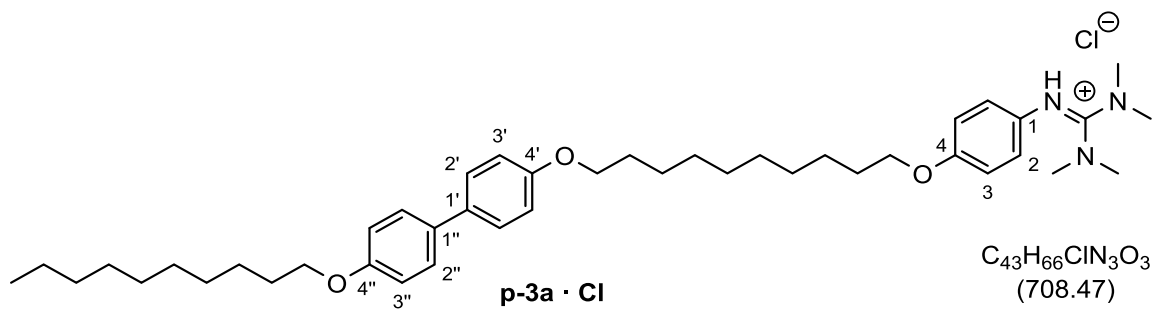
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 Operator wo/tri
 Instrument micrOTOF-Q 43

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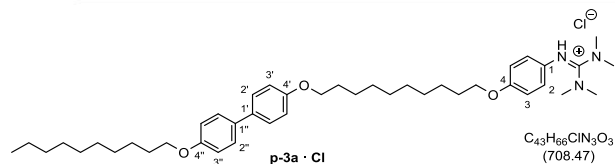
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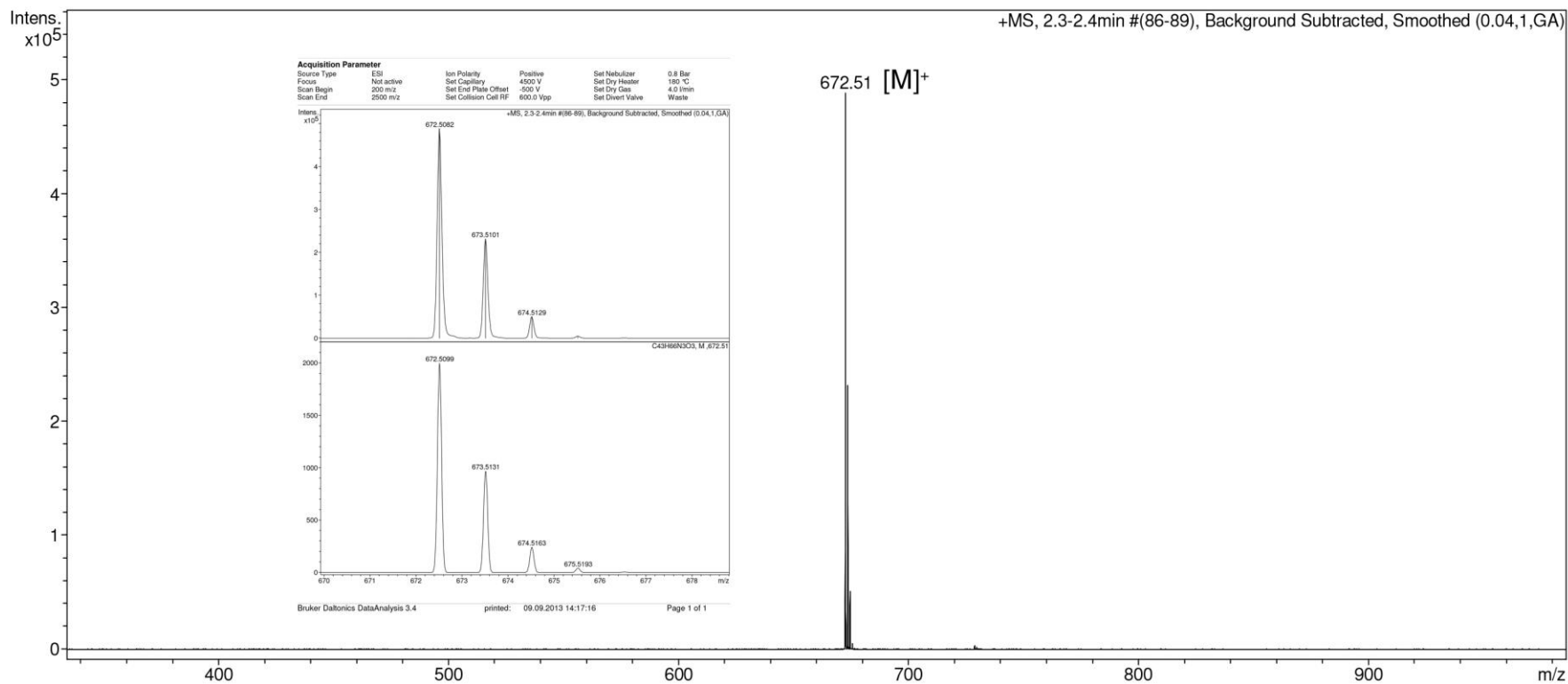
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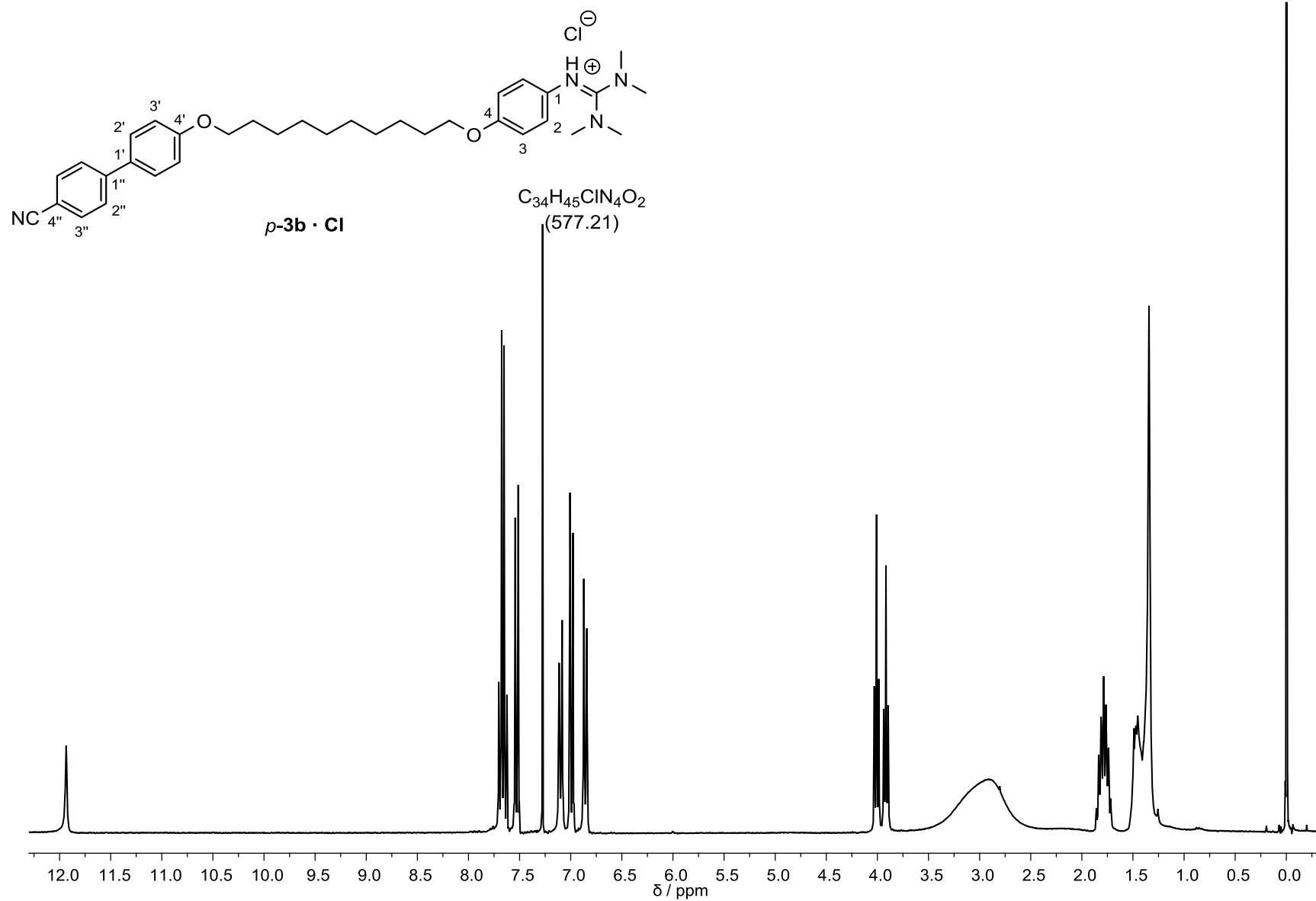
Operator wo/tri

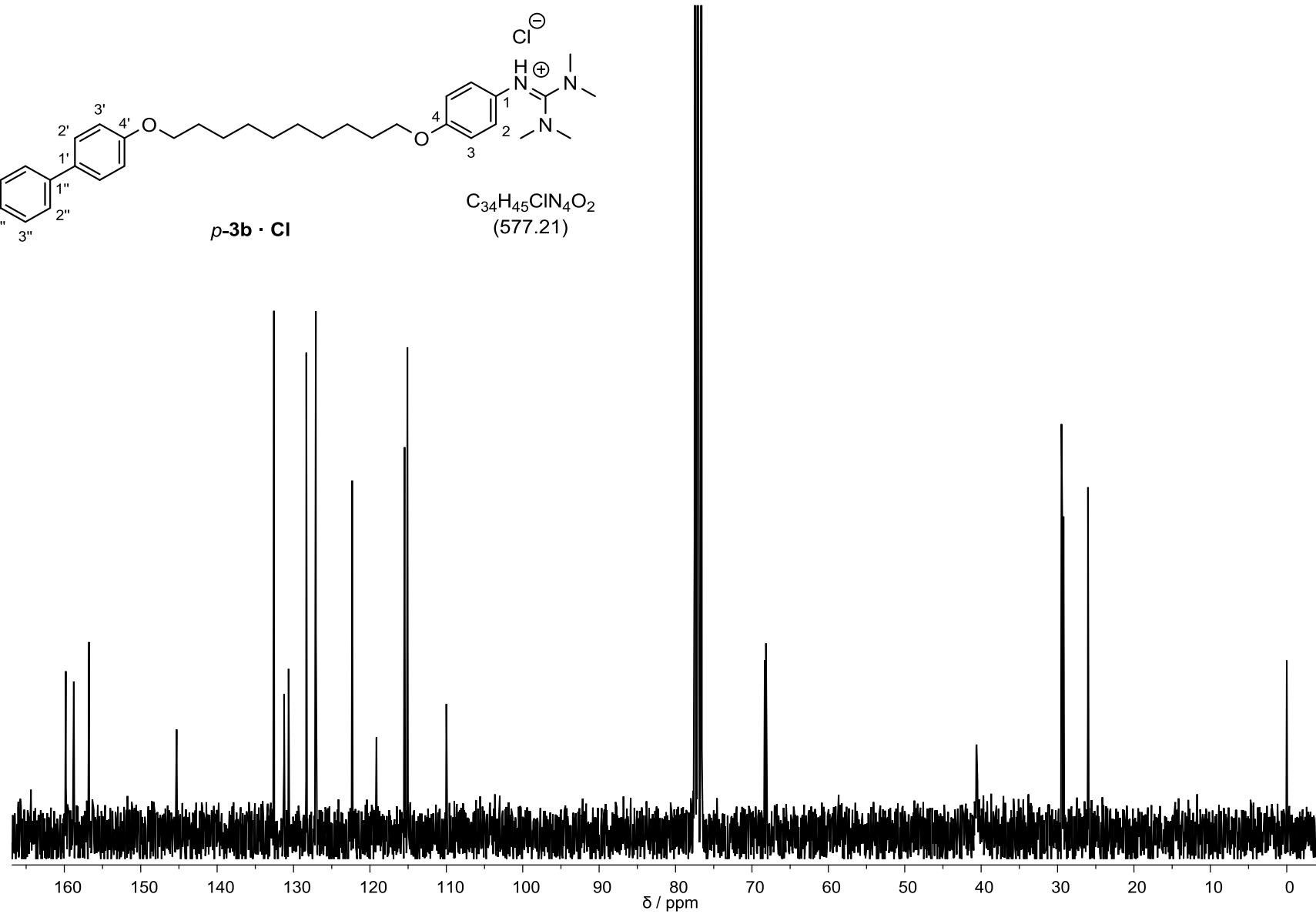
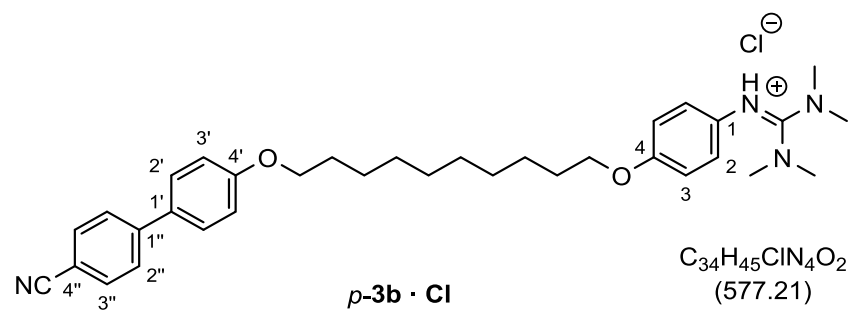
Instrument micrOTOF-Q 43

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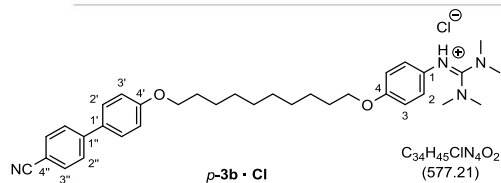
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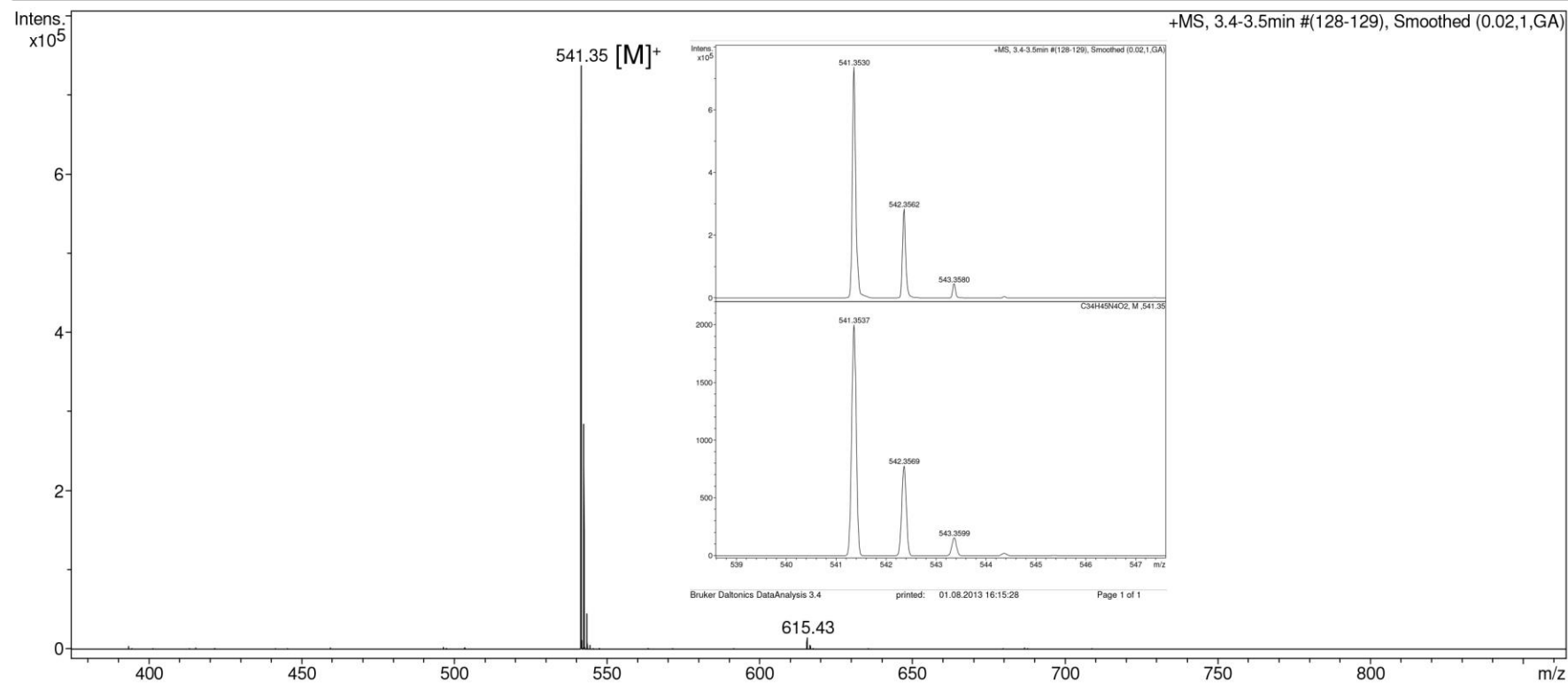
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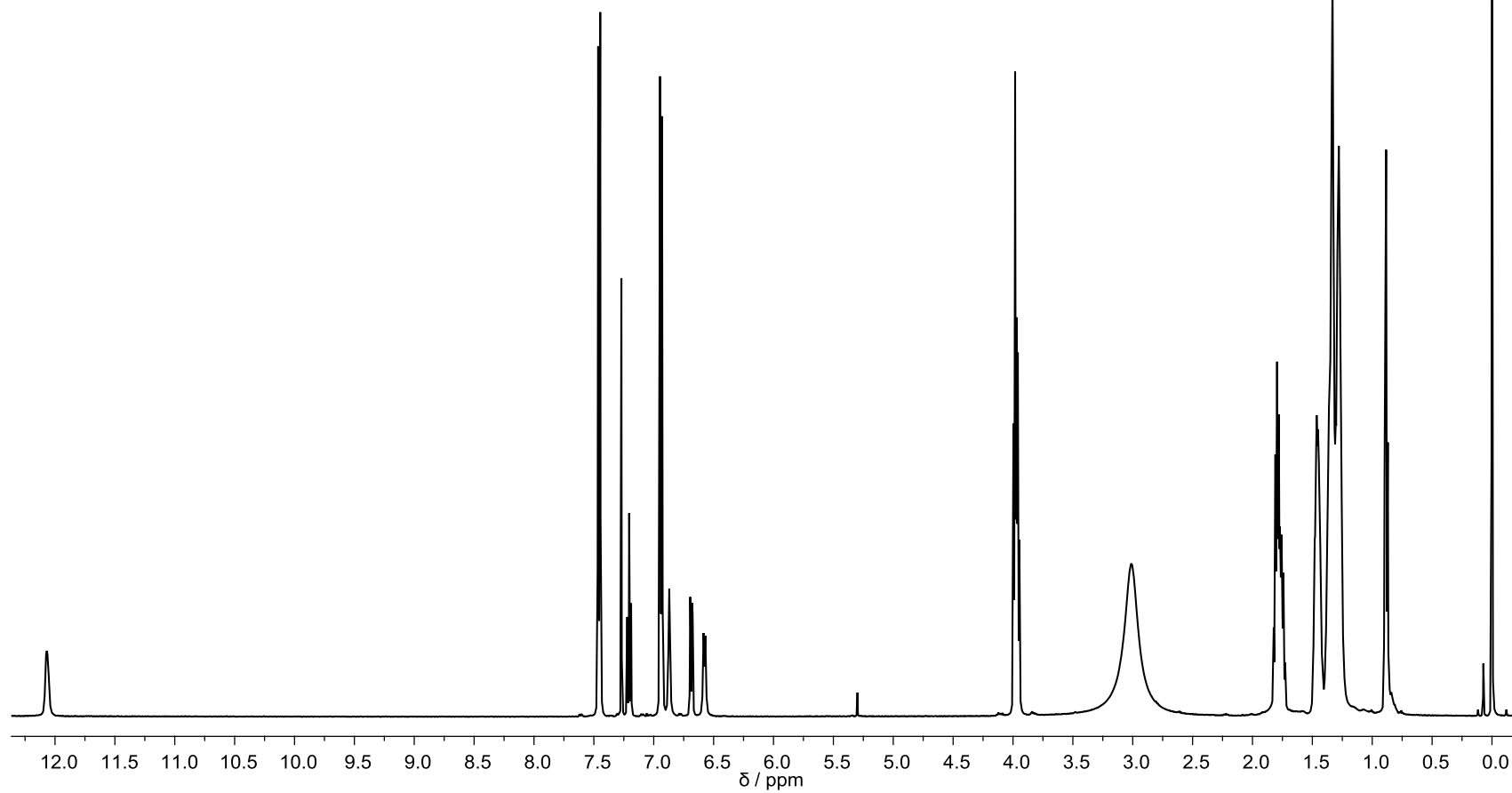
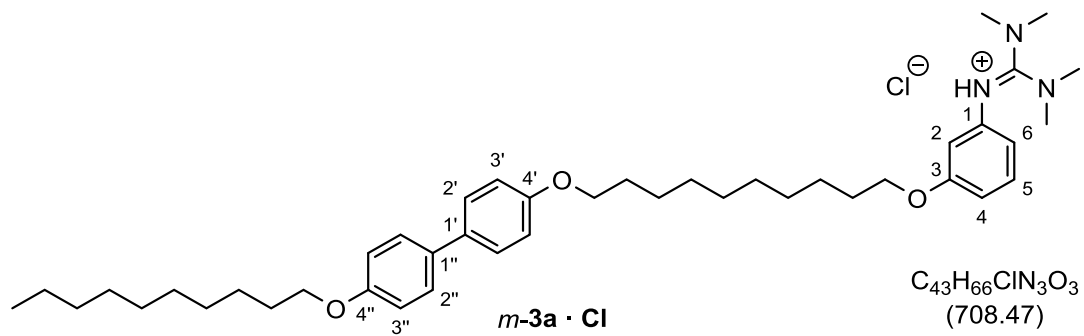


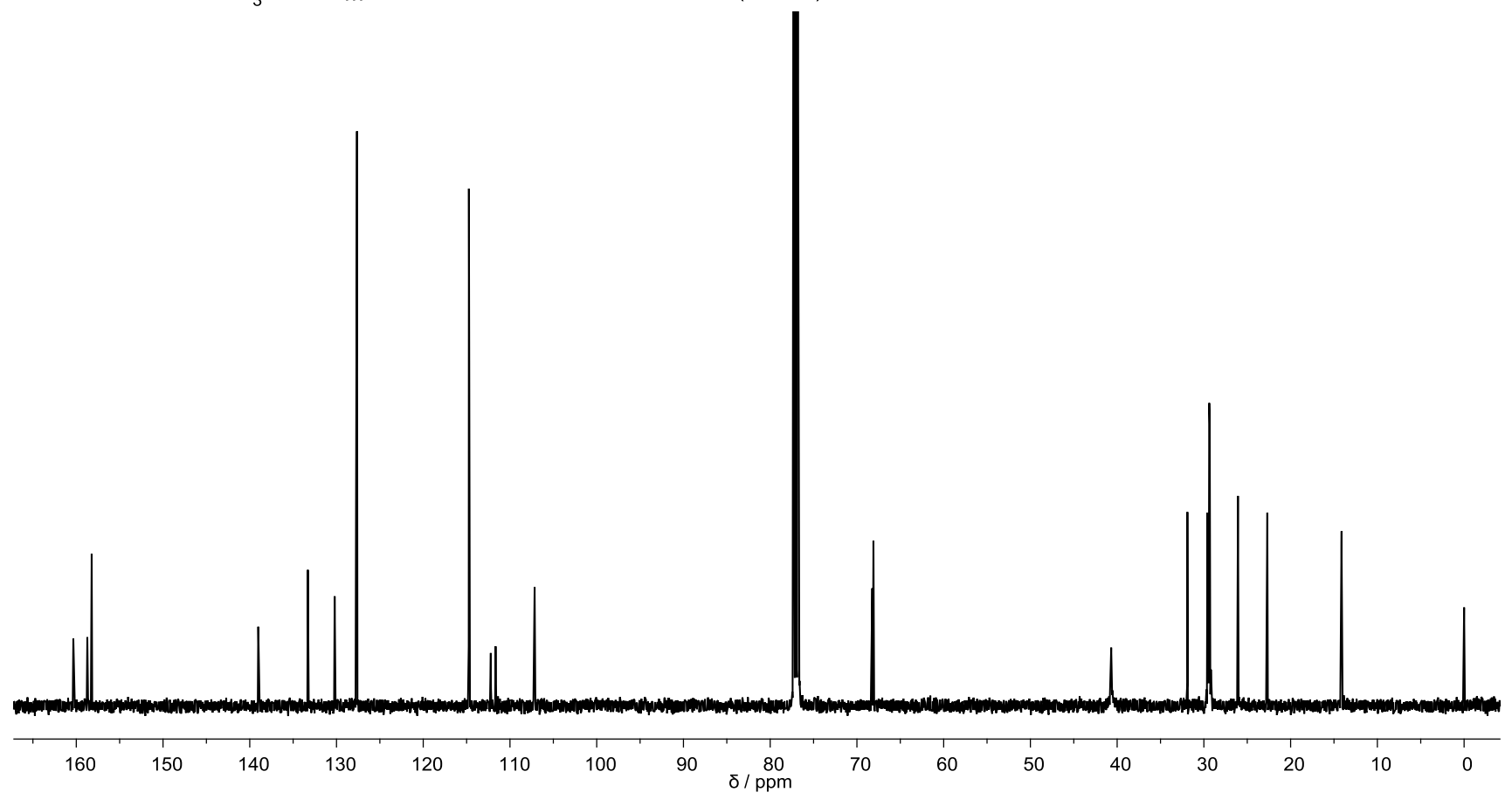
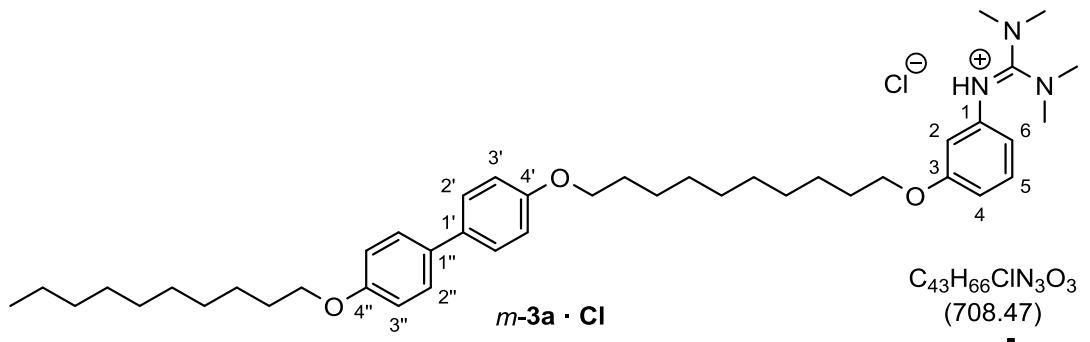
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 Operator wo/tri
 Instrument micrOTOF-Q 43

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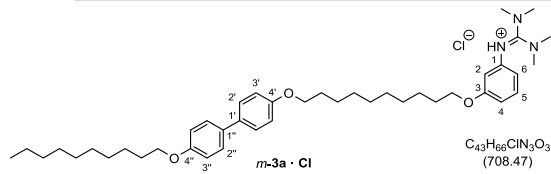
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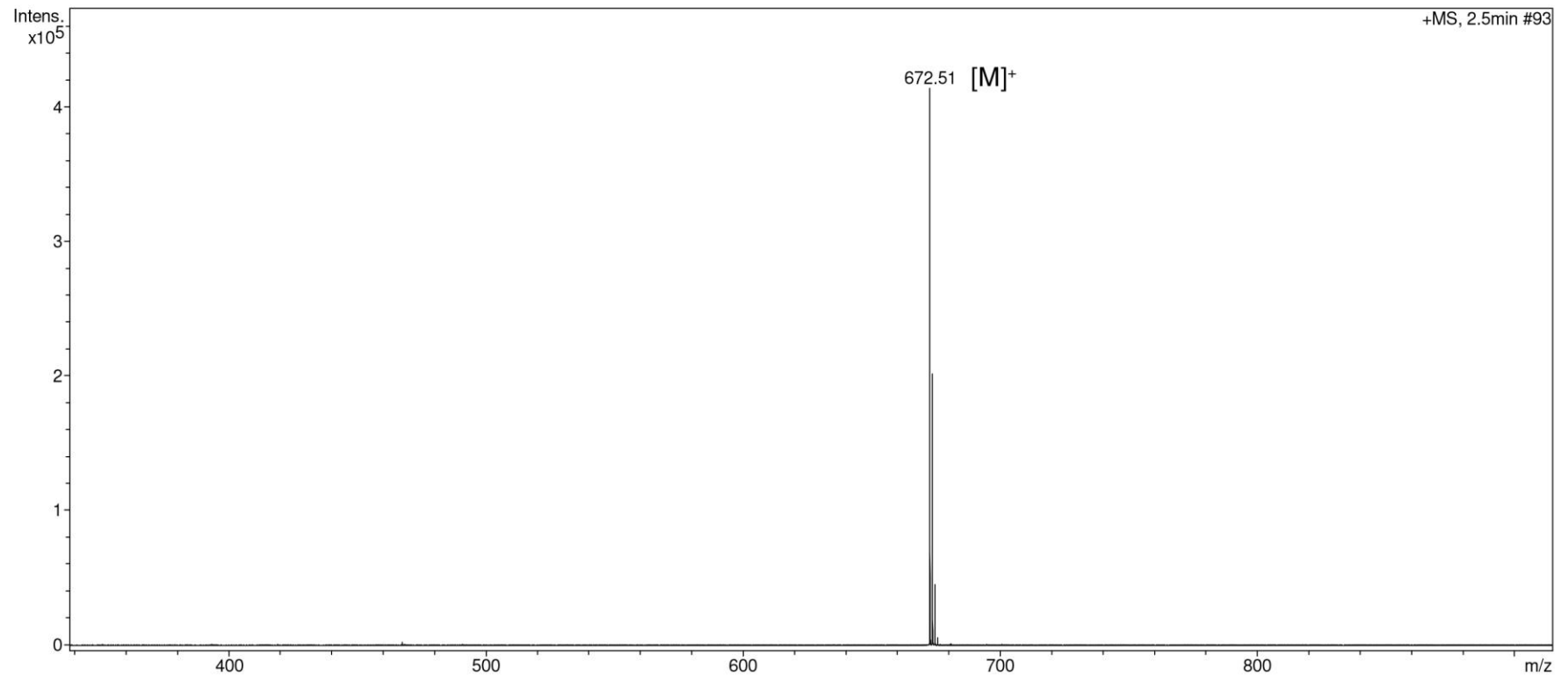


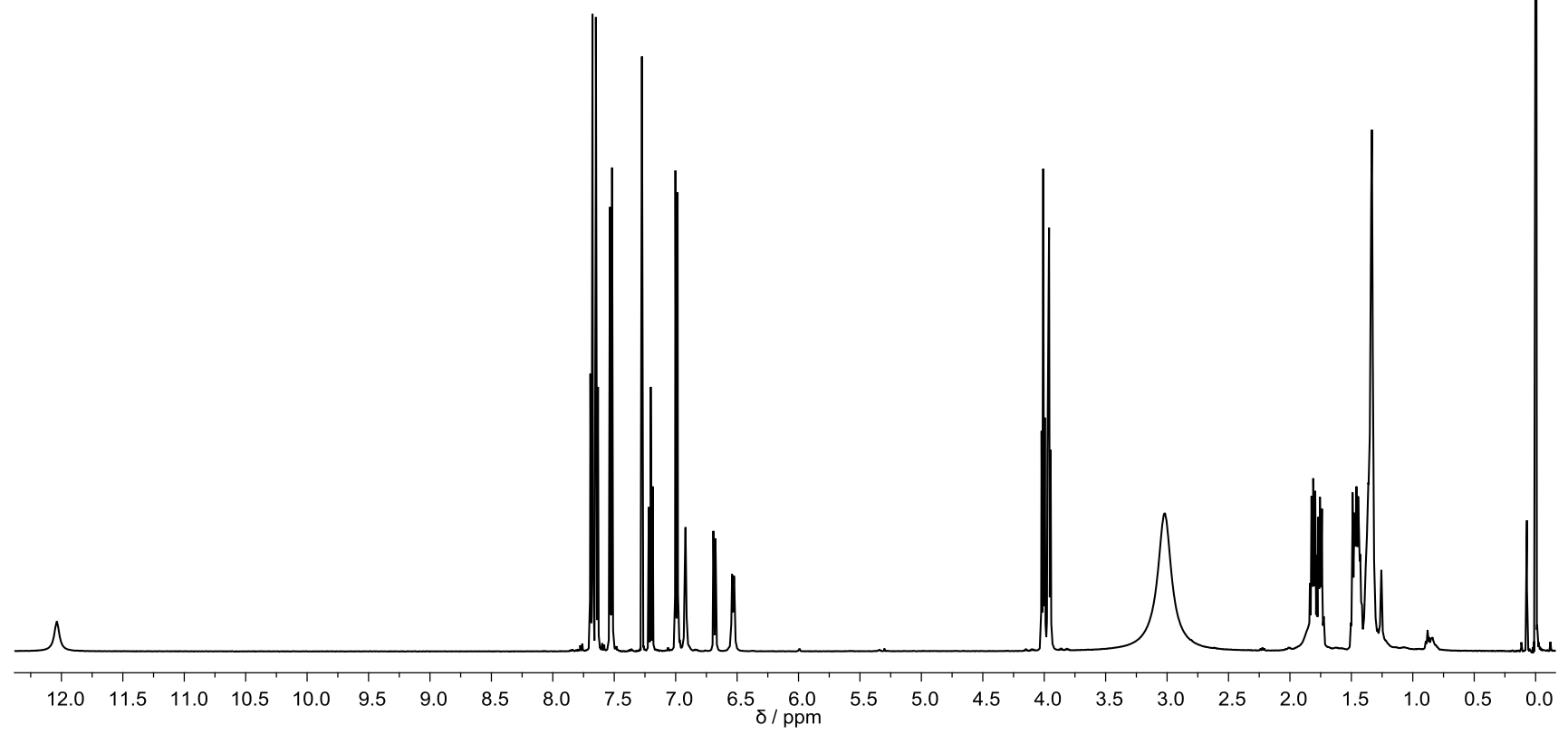
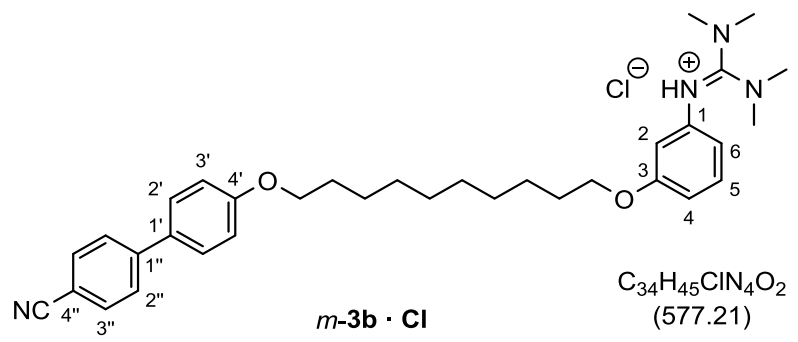
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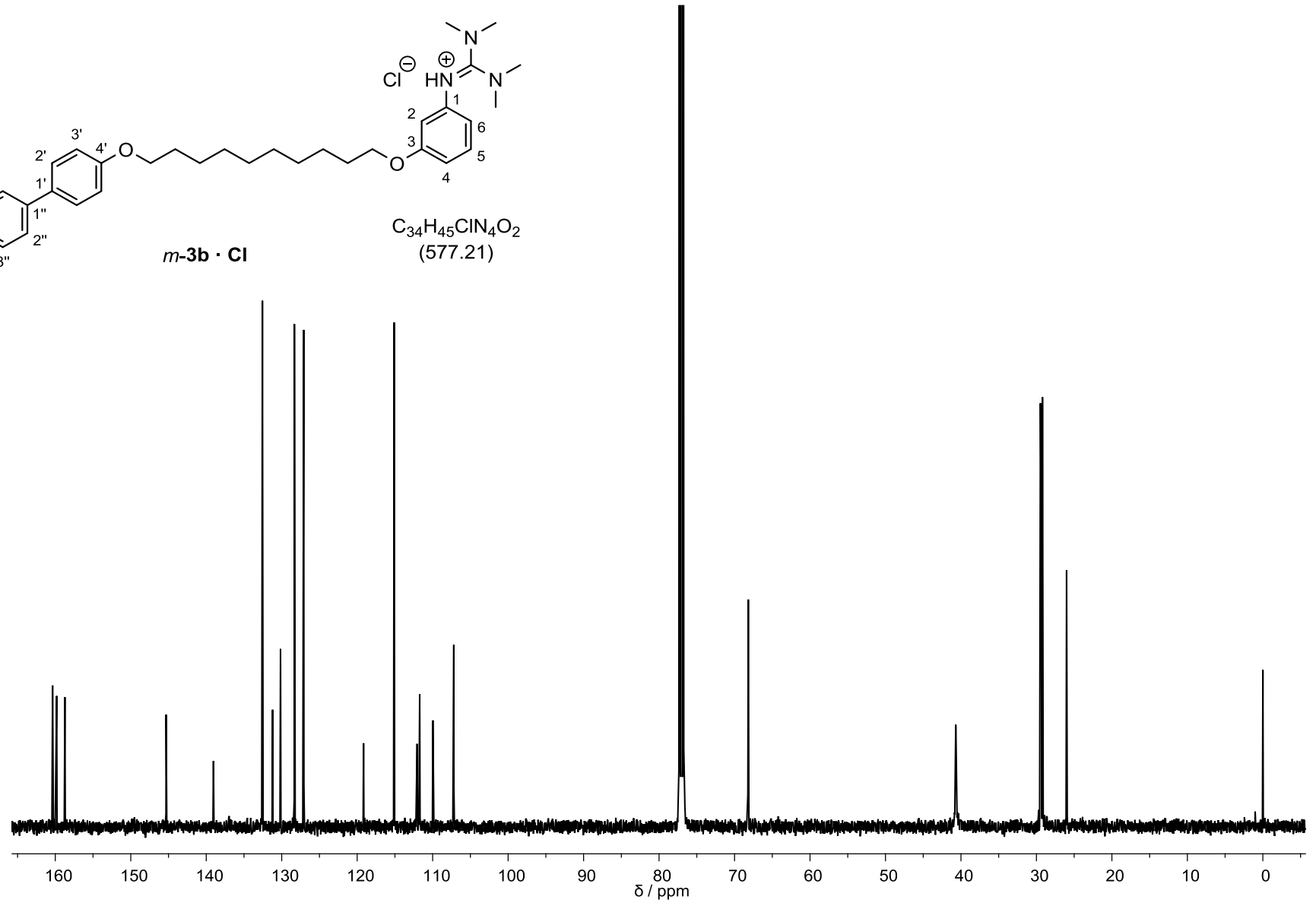
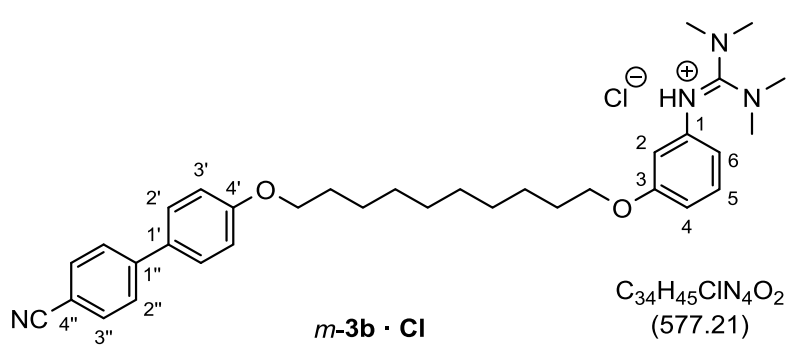
Operator wo/tri
Instrument micrOTOF-Q 43

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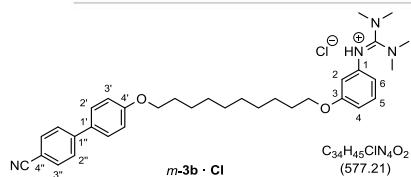
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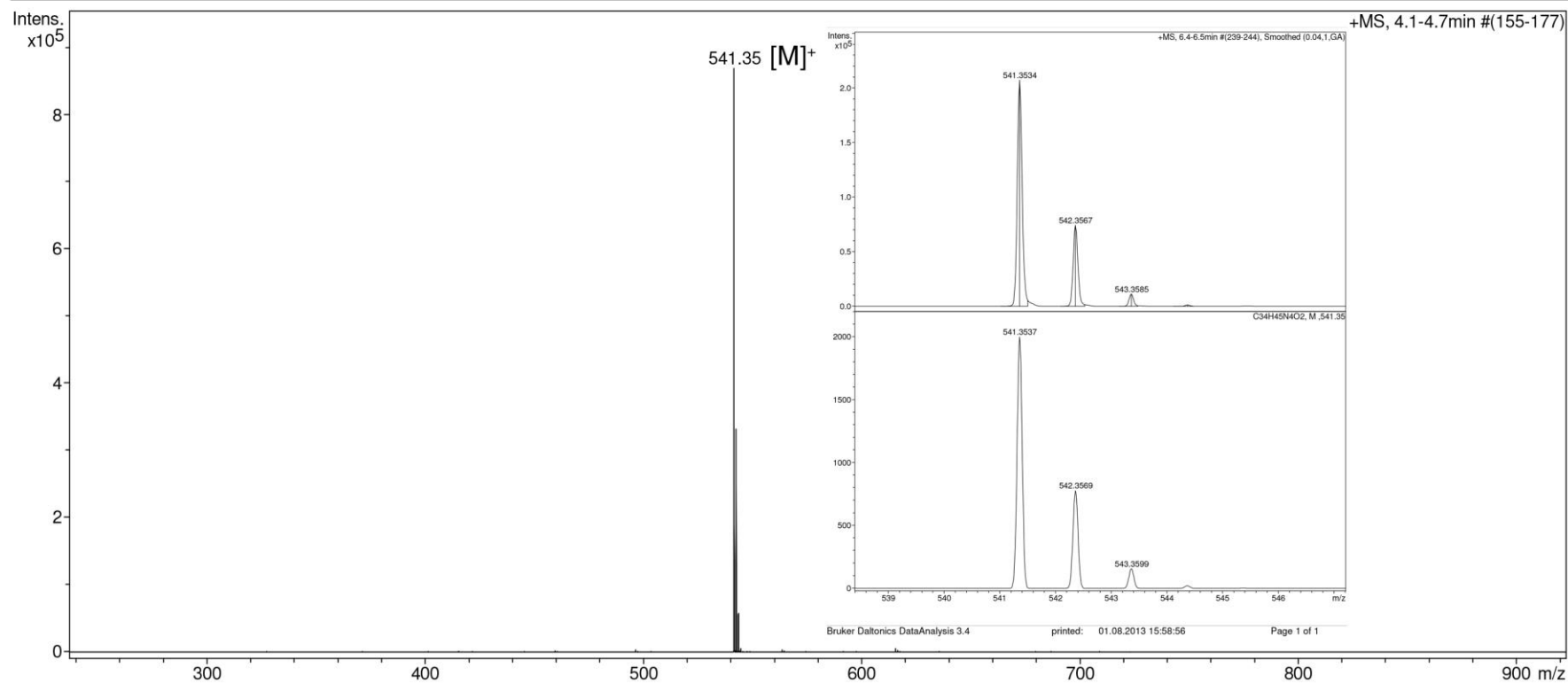
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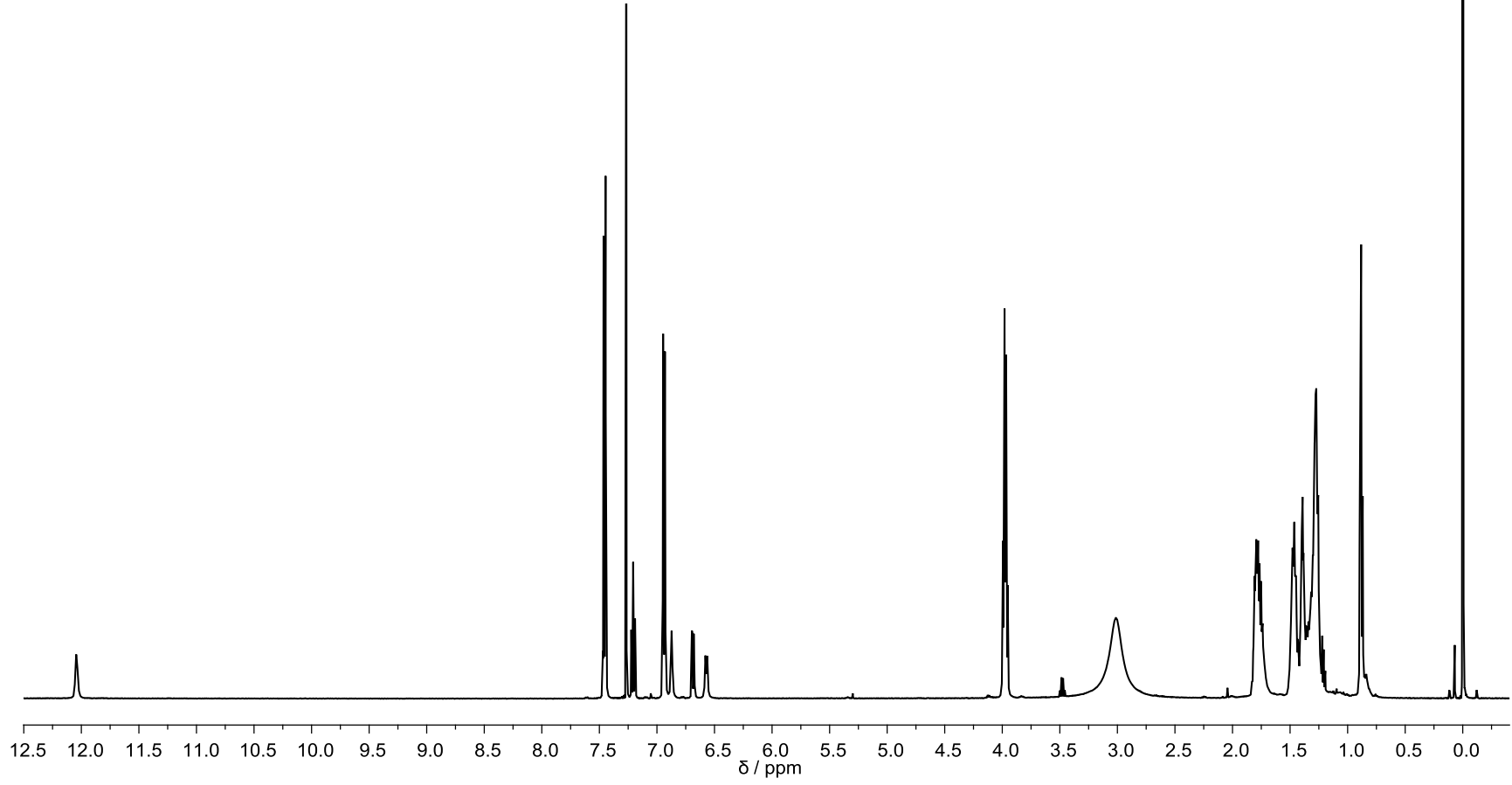
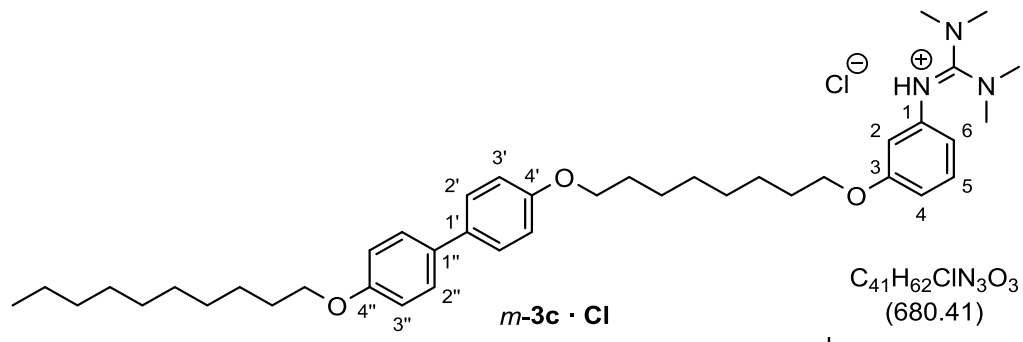


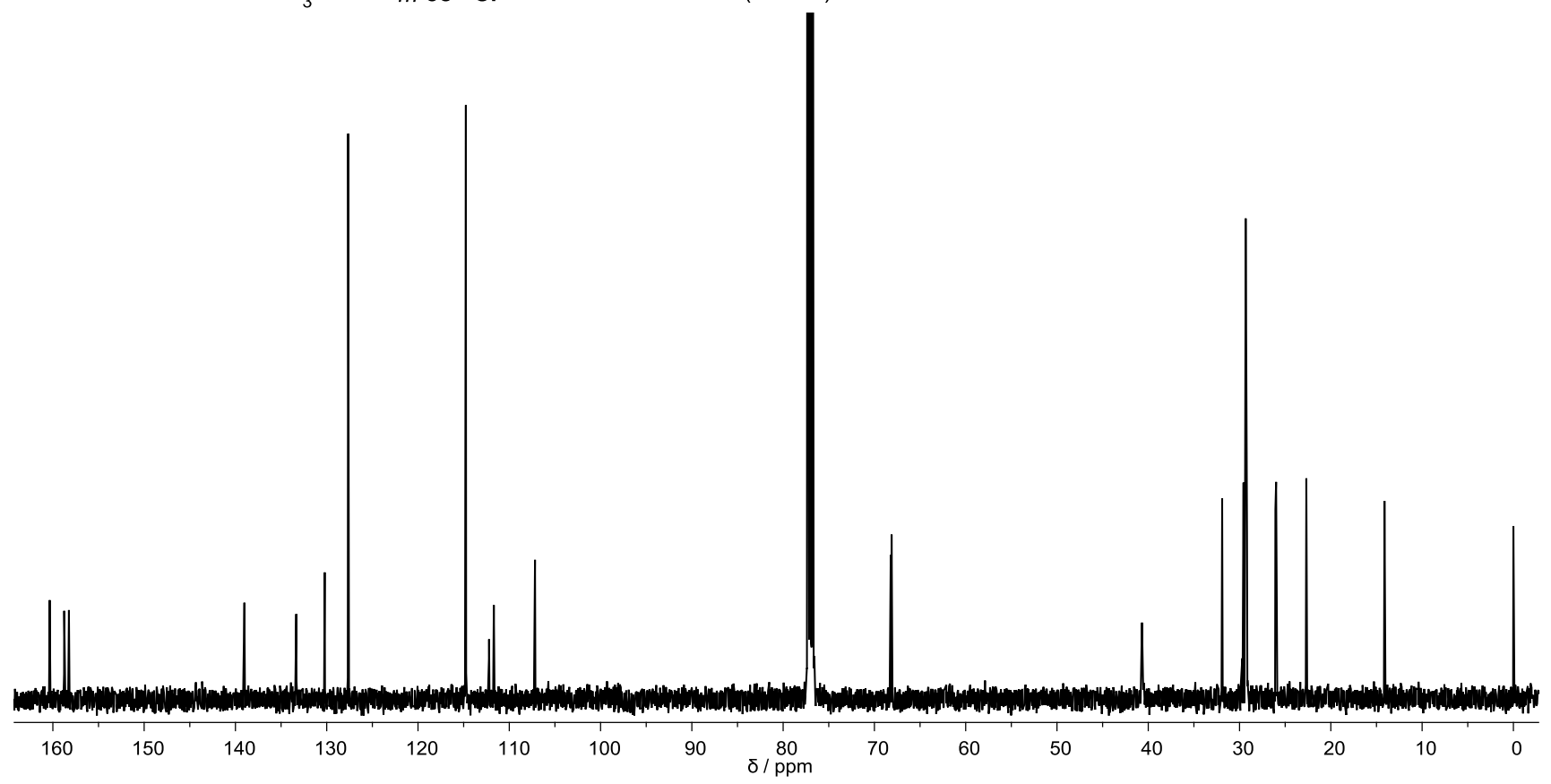
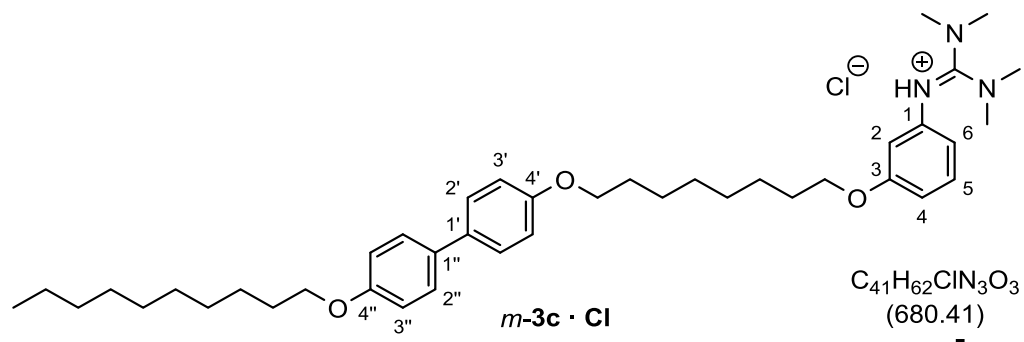
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 Operator wo/tri
 Instrument micrOTOF-Q 43

Acquisition Parameter

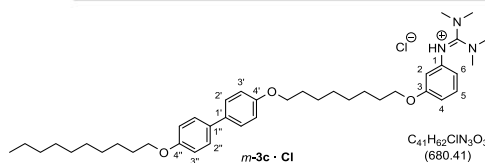
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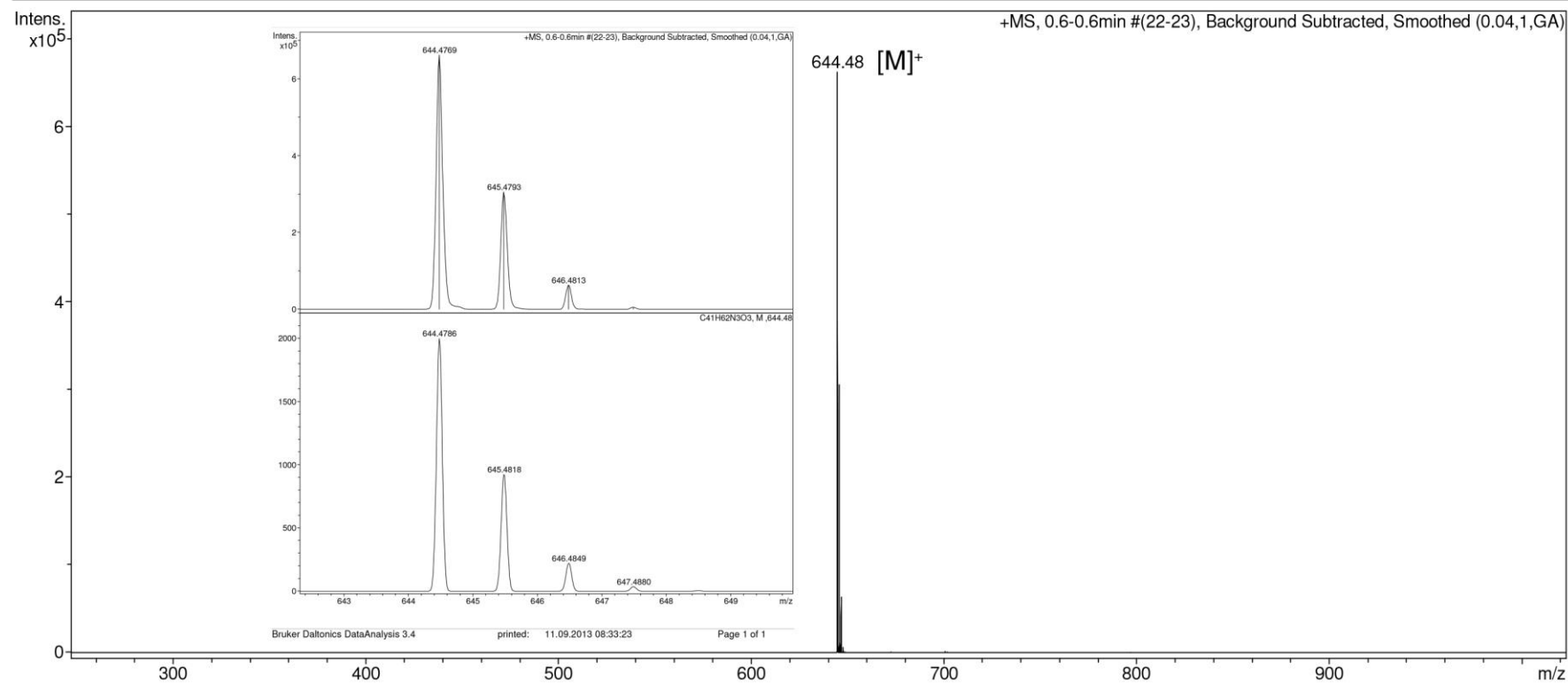
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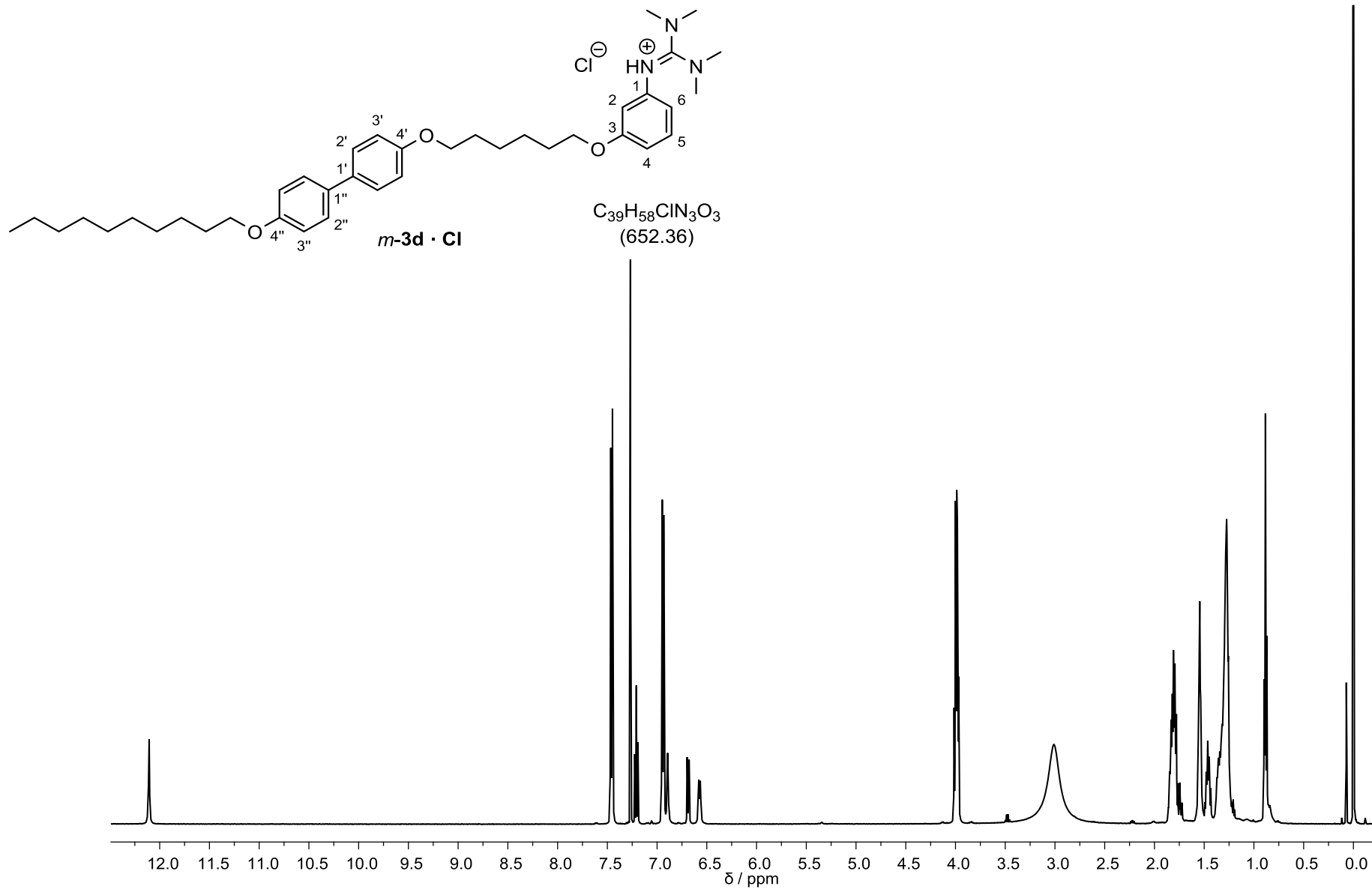


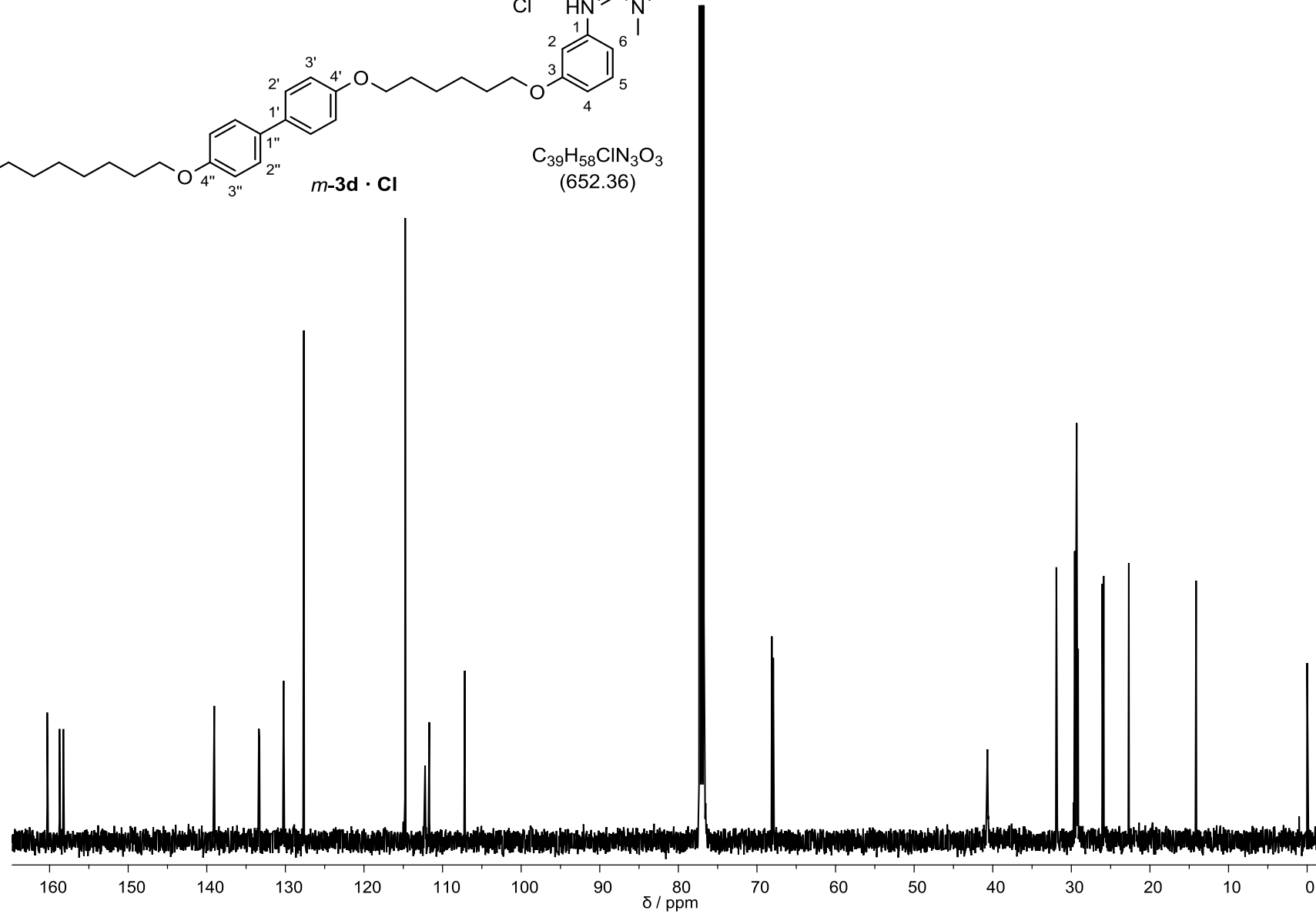
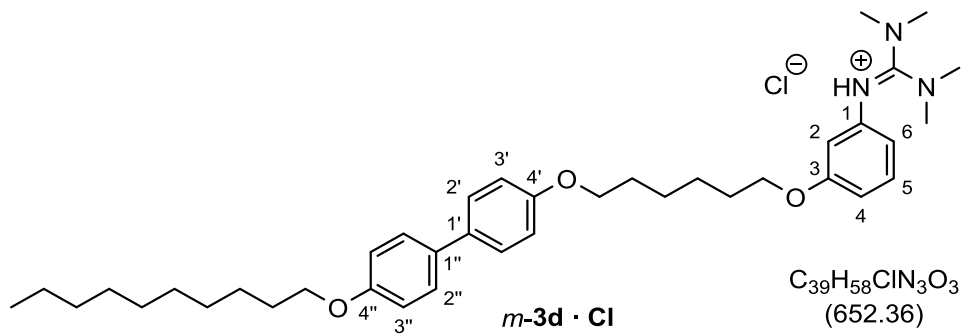
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 Operator wo/tri
 Instrument micrOTOF-Q 43

Acquisition Parameter

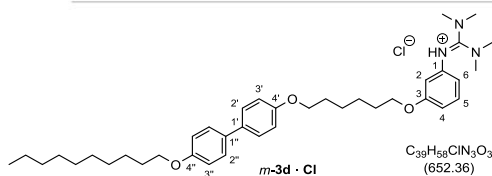
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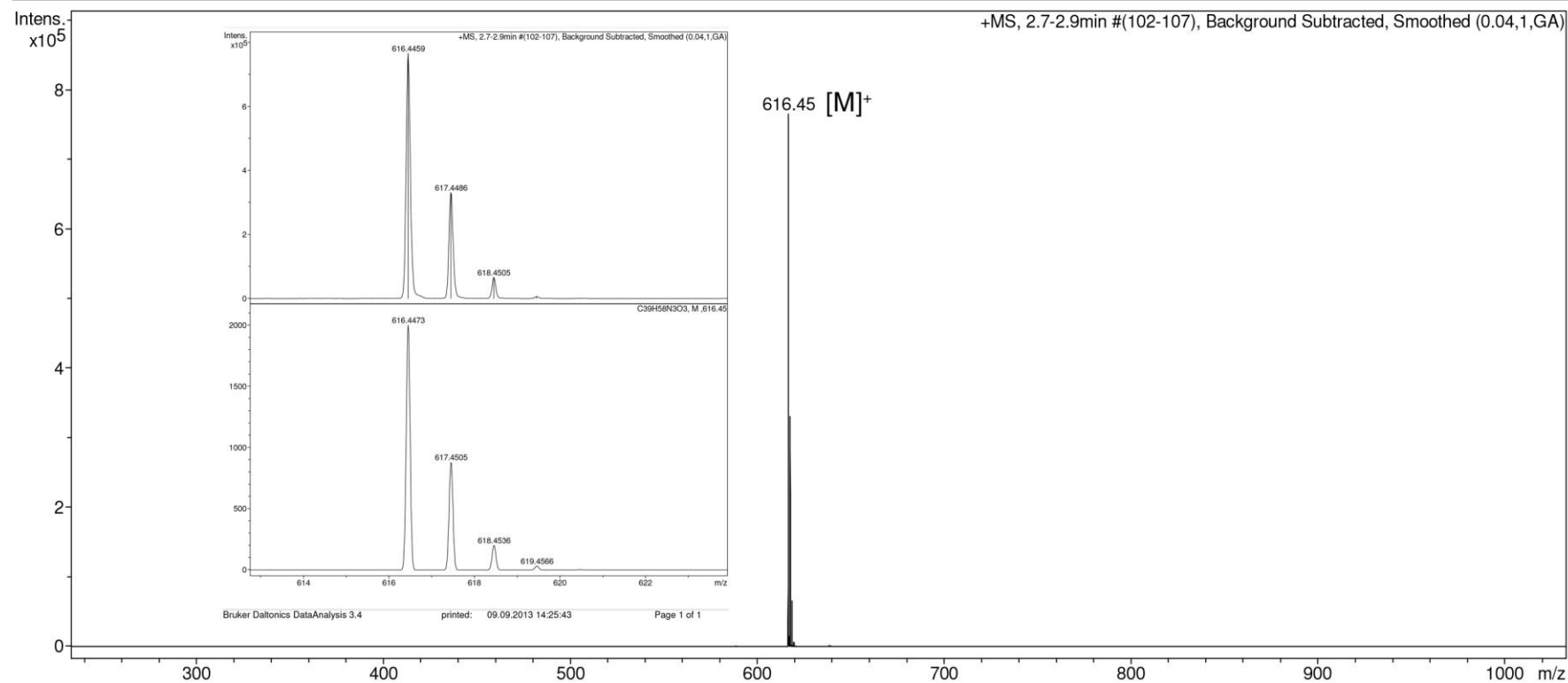
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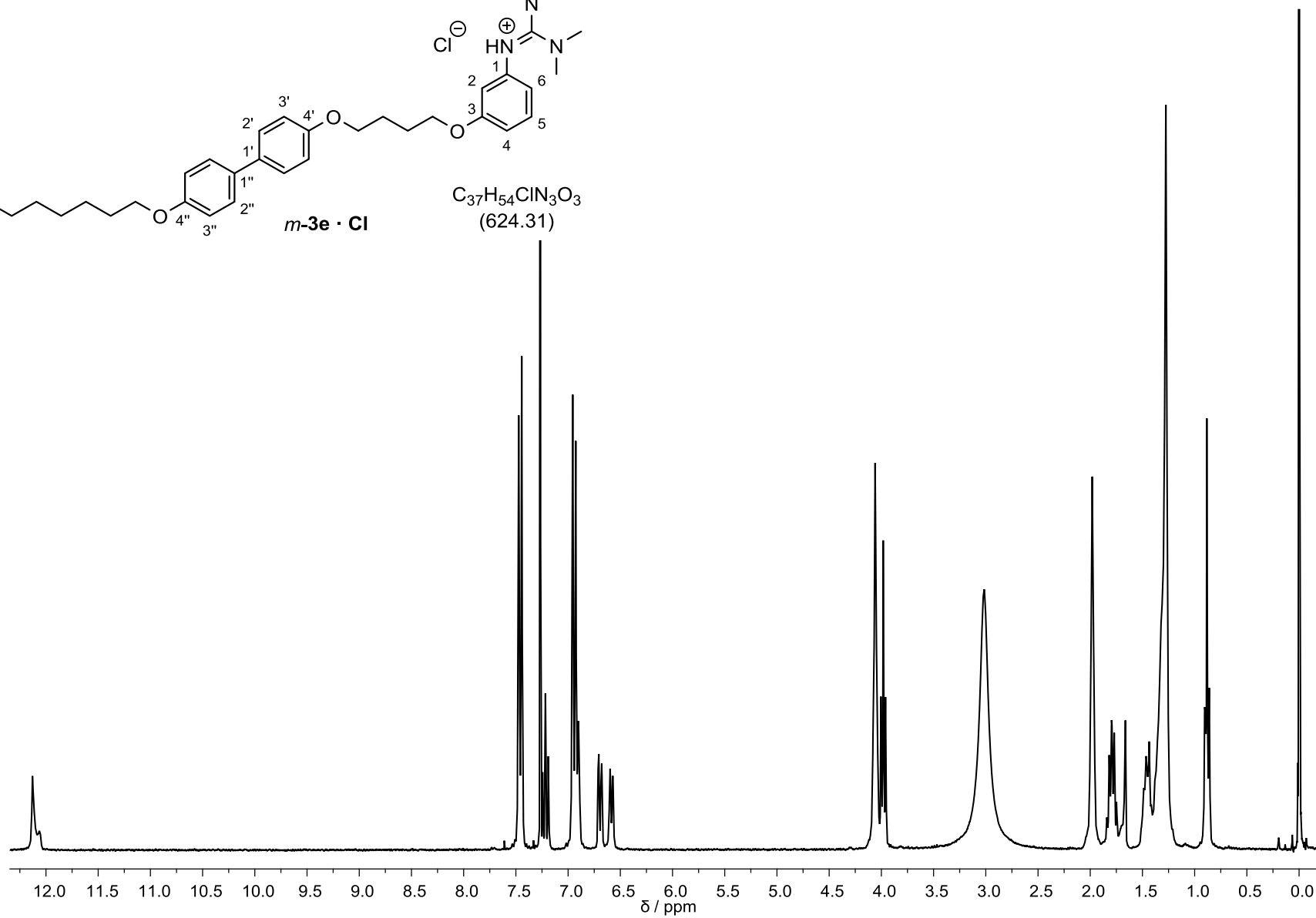
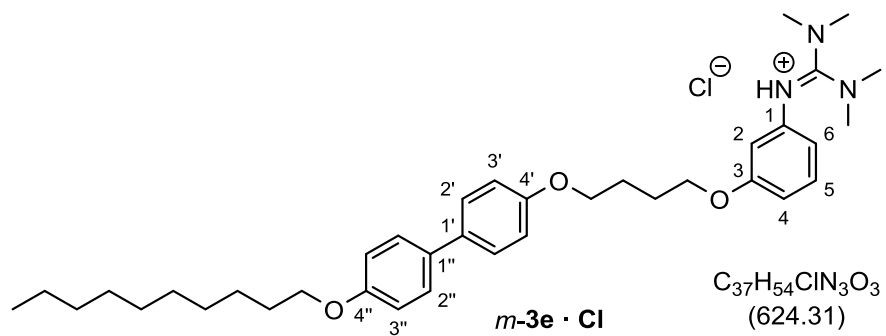


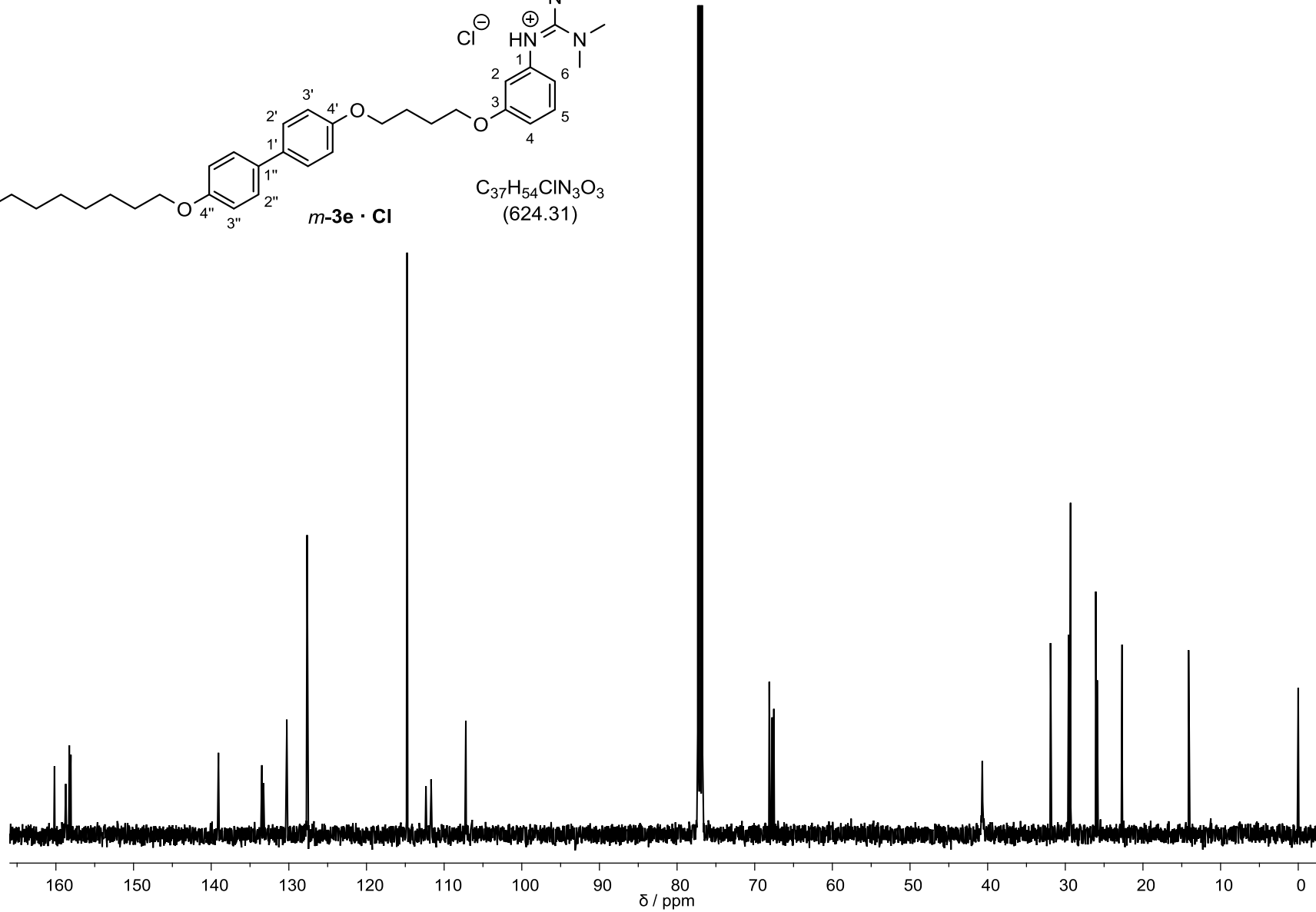
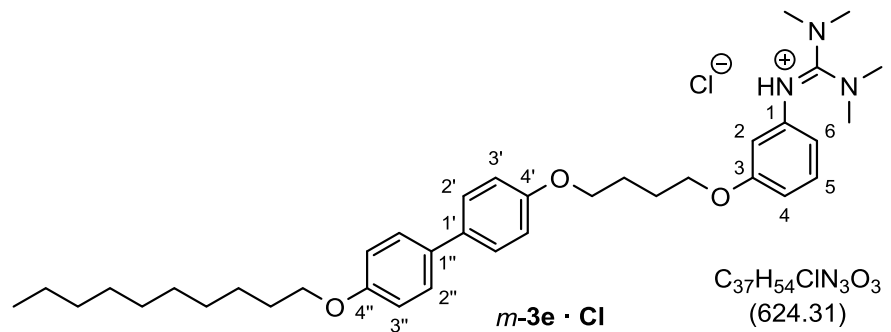
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 Operator wo/tri
 Instrument micrOTOF-Q 43

Acquisition Parameter

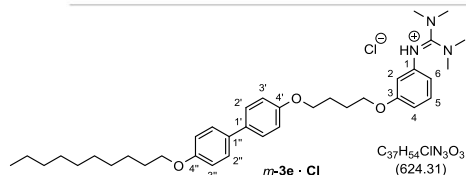
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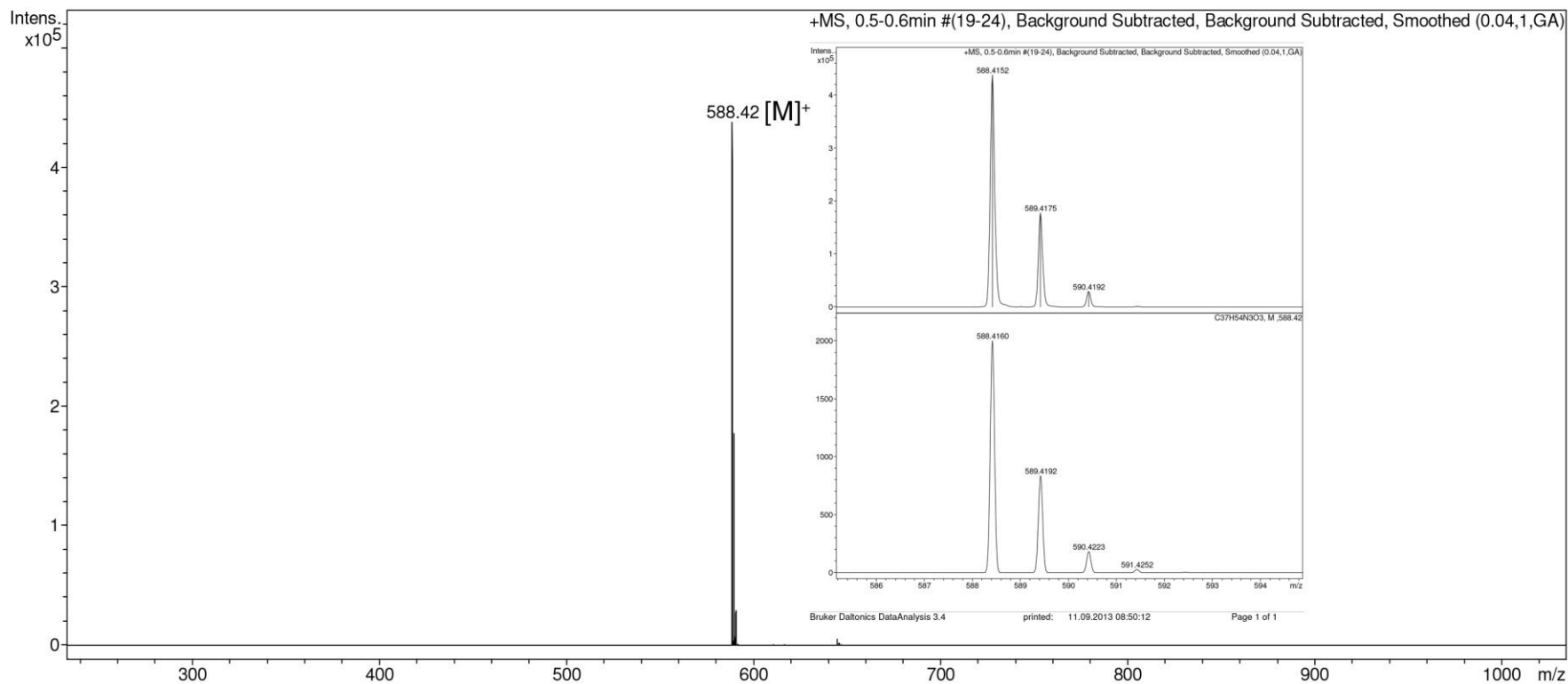
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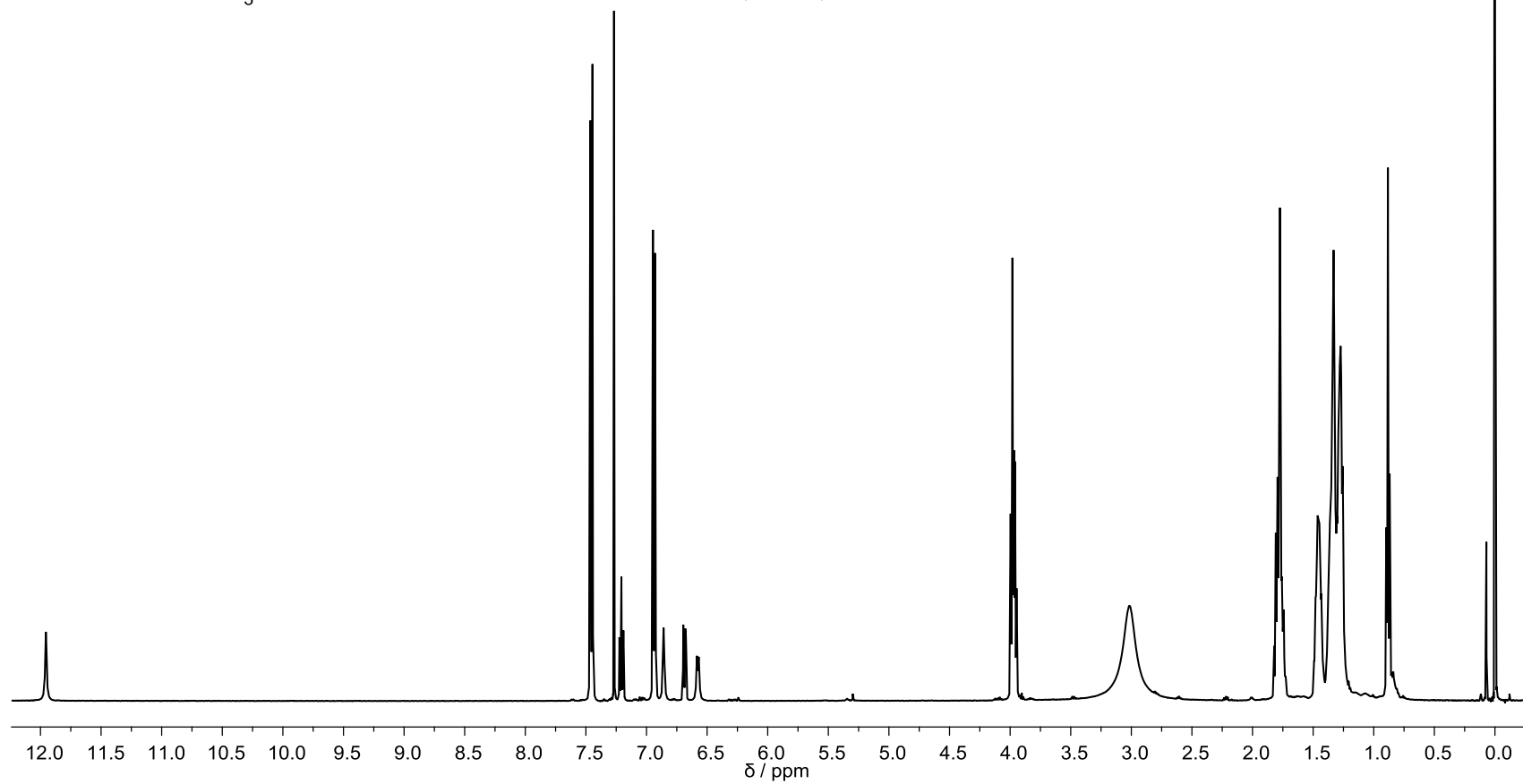
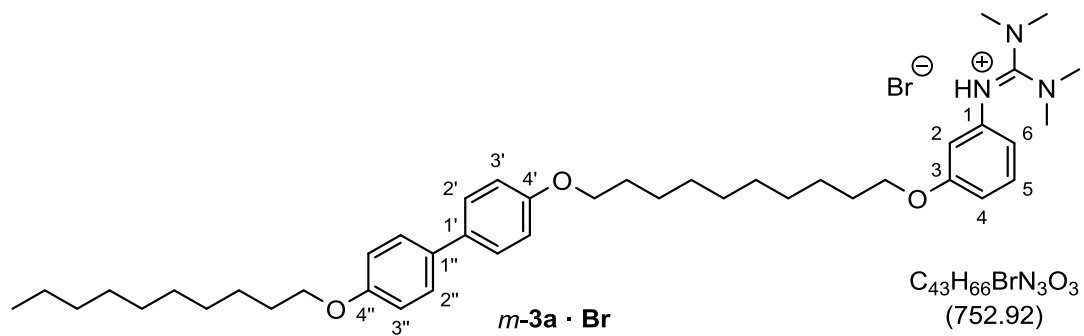


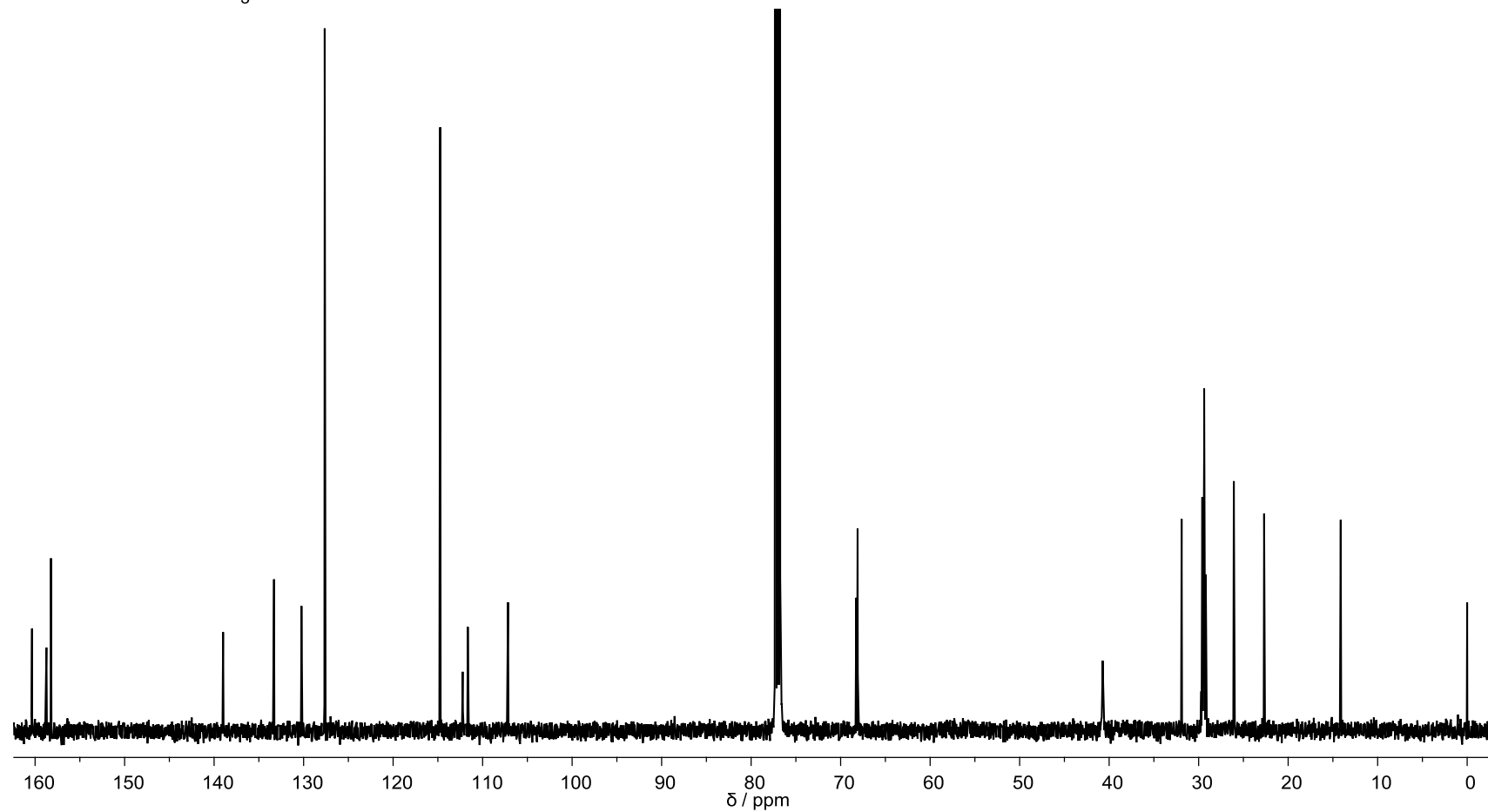
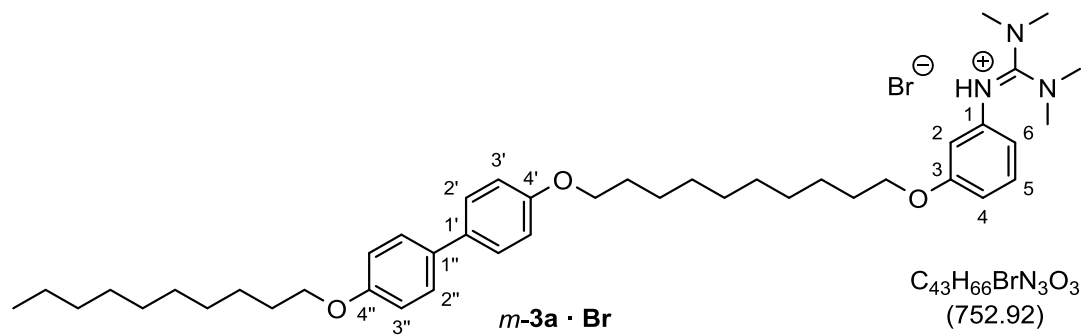
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 Operator wo/tri
 Instrument micrOTOF-Q 43

Acquisition Parameter

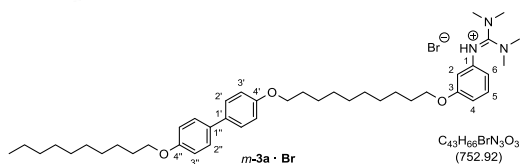
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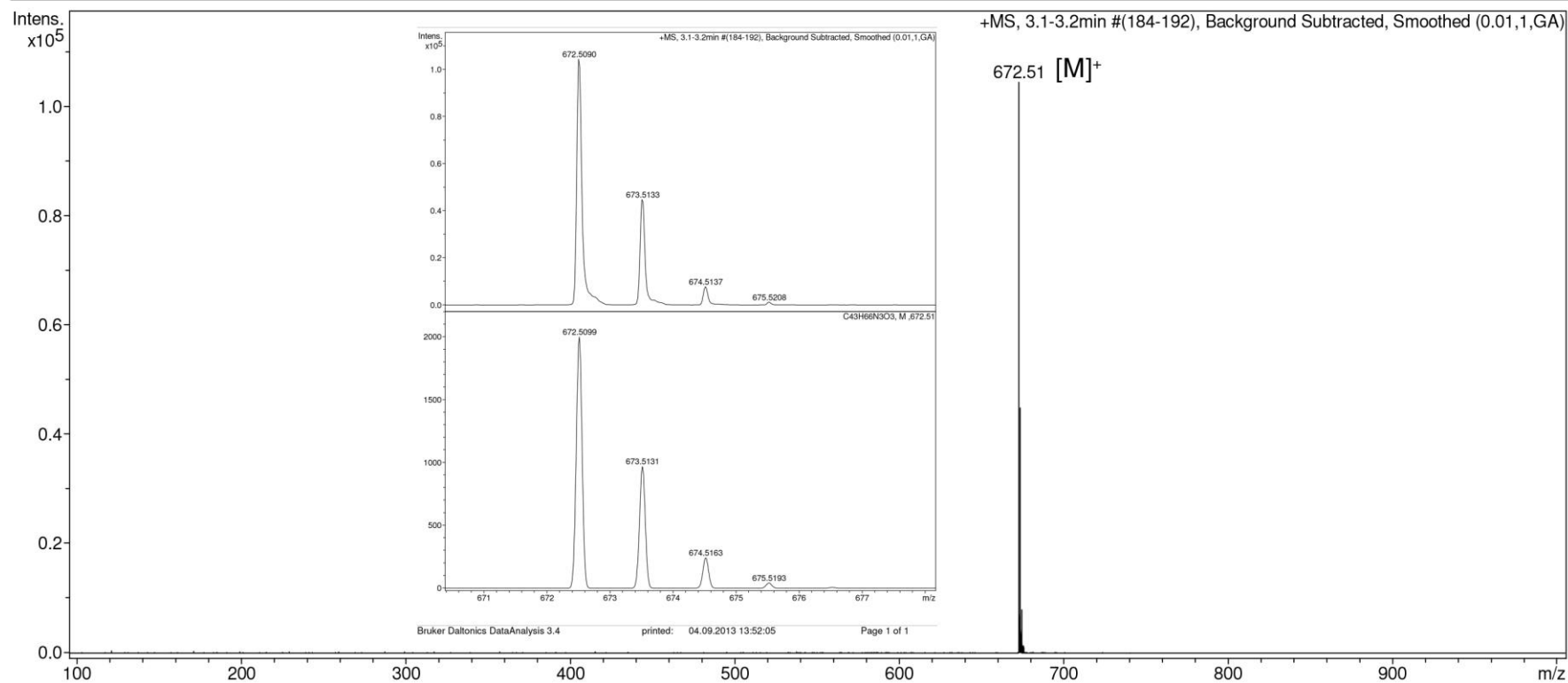
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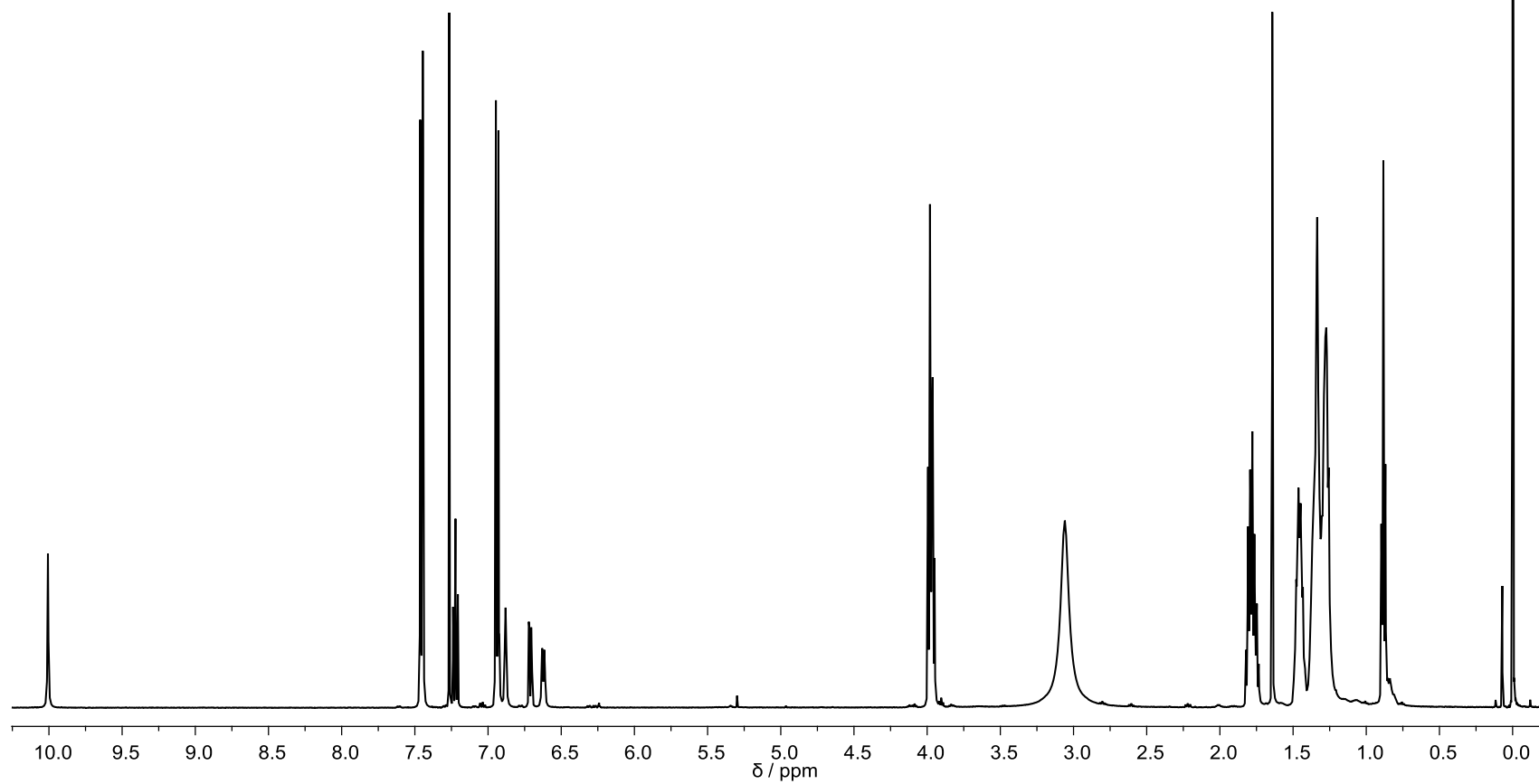
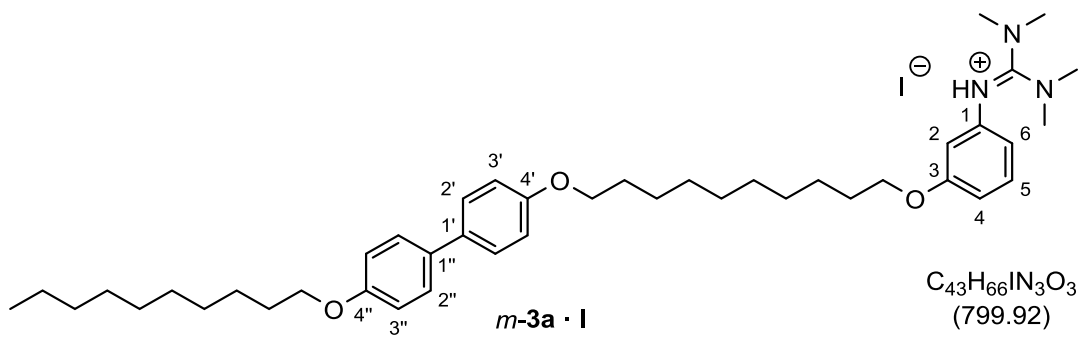


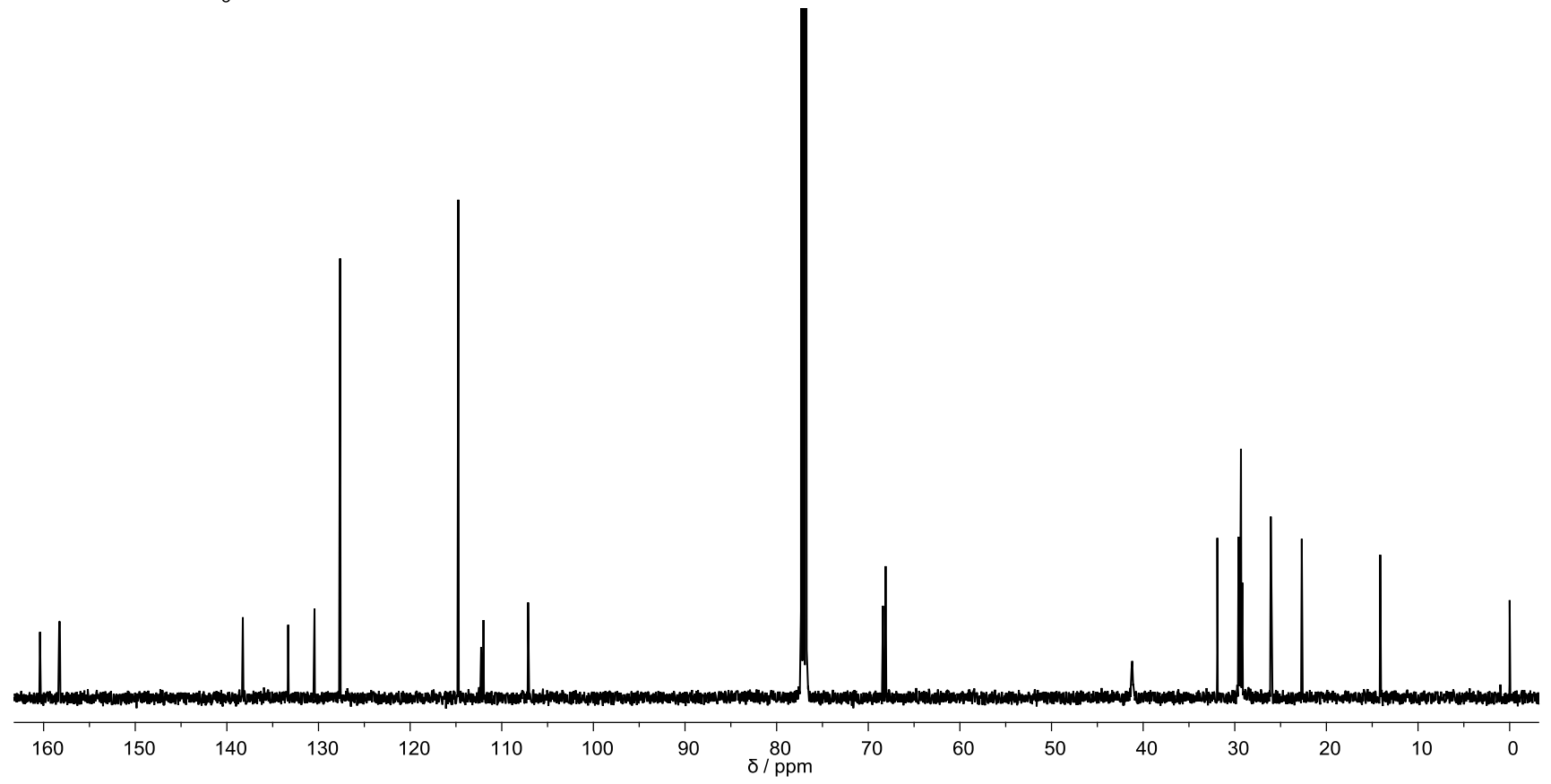
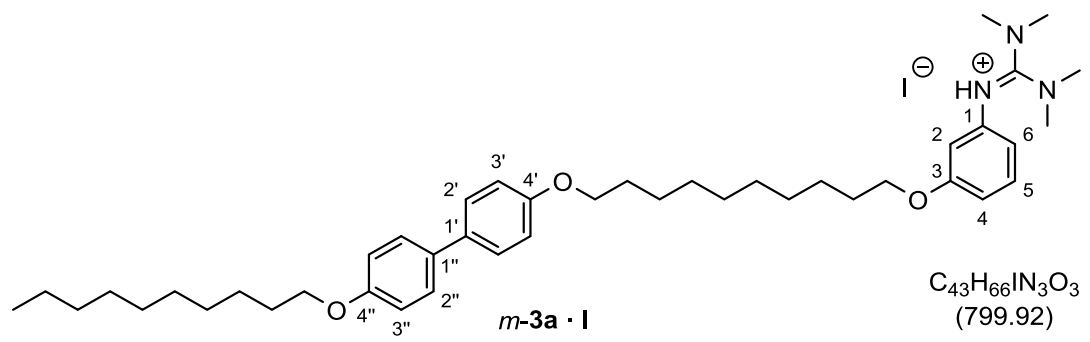
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 Operator wo/tri
 Instrument micrOTOF-Q 43

Acquisition Parameter

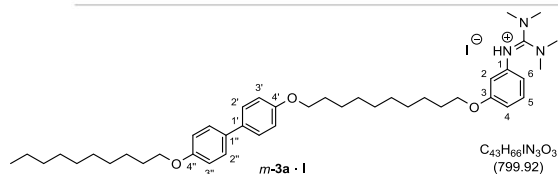
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Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste







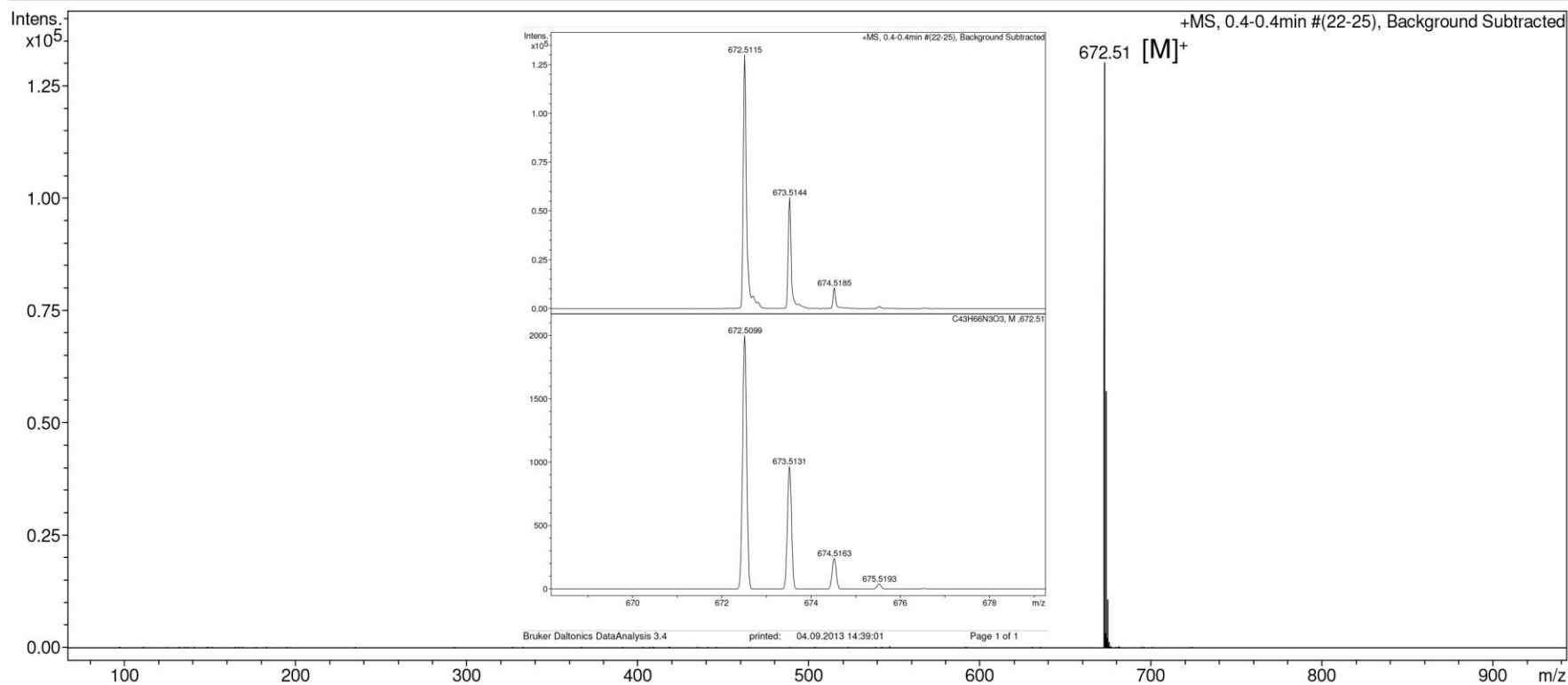
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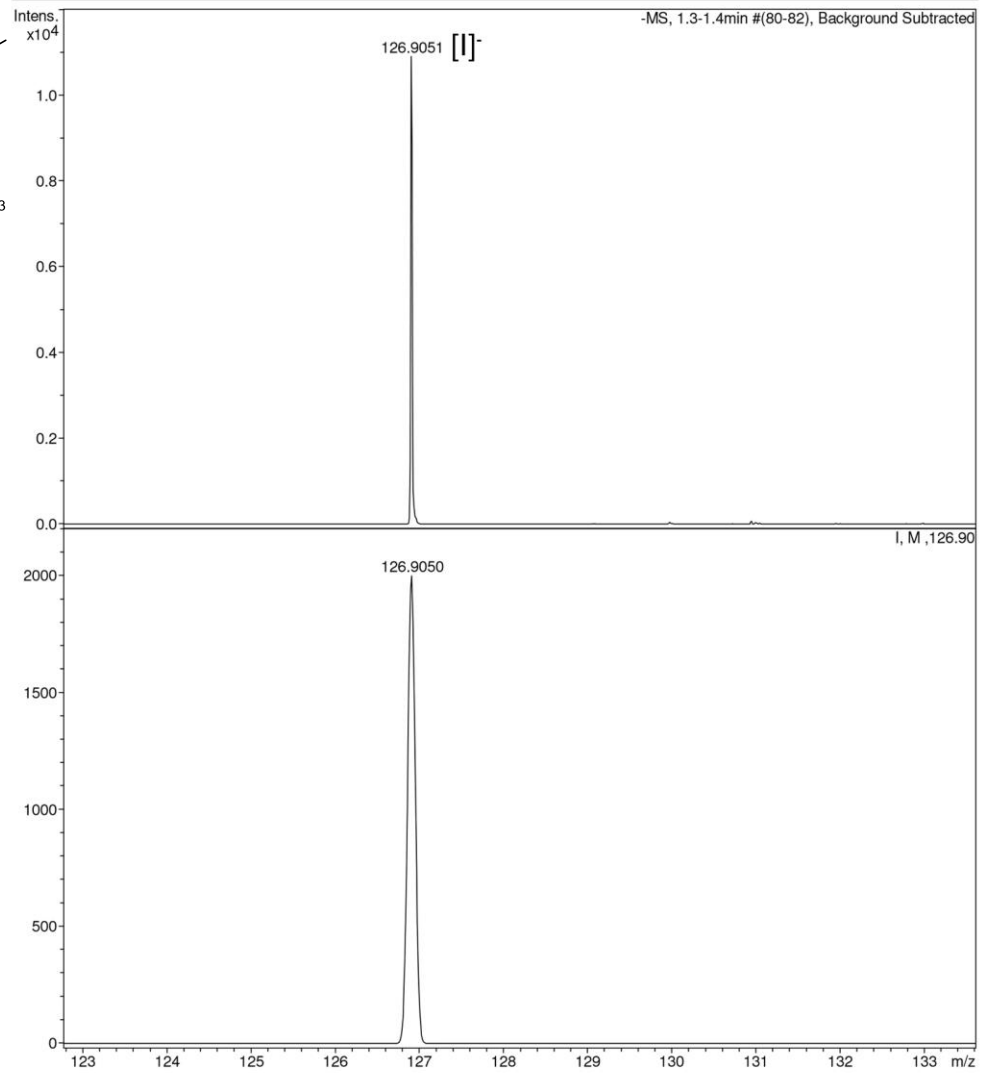
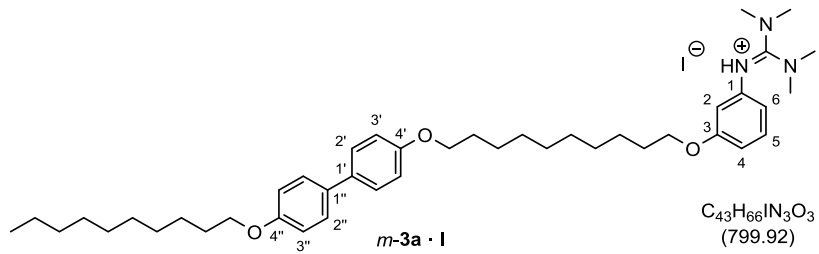


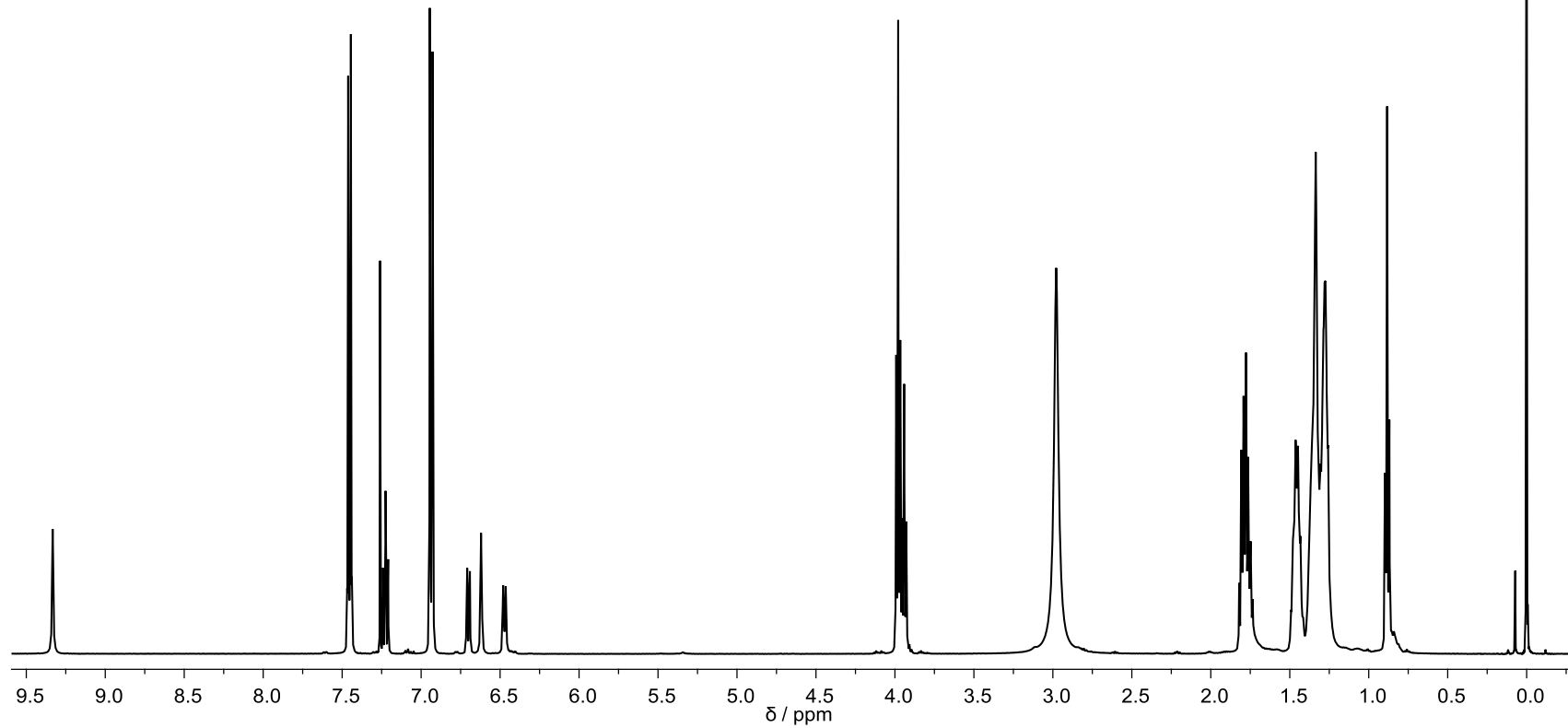
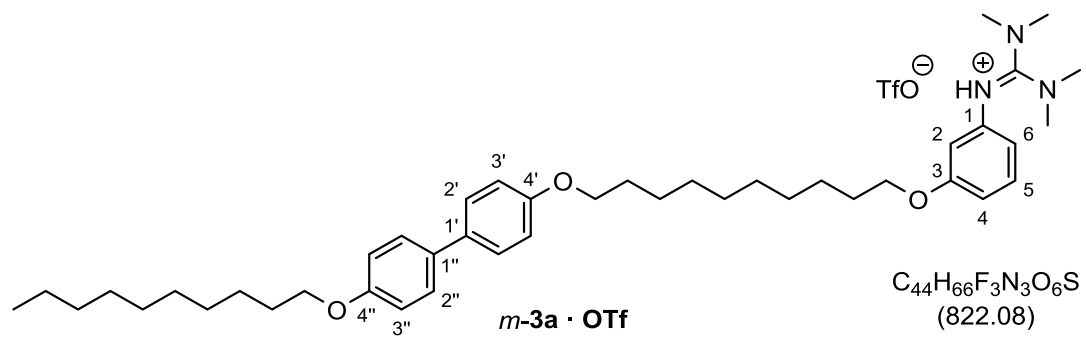
Acquisition Date 04.09.2013 14:31:47
 Operator wo/tri
 Instrument micrOTOF-Q 43

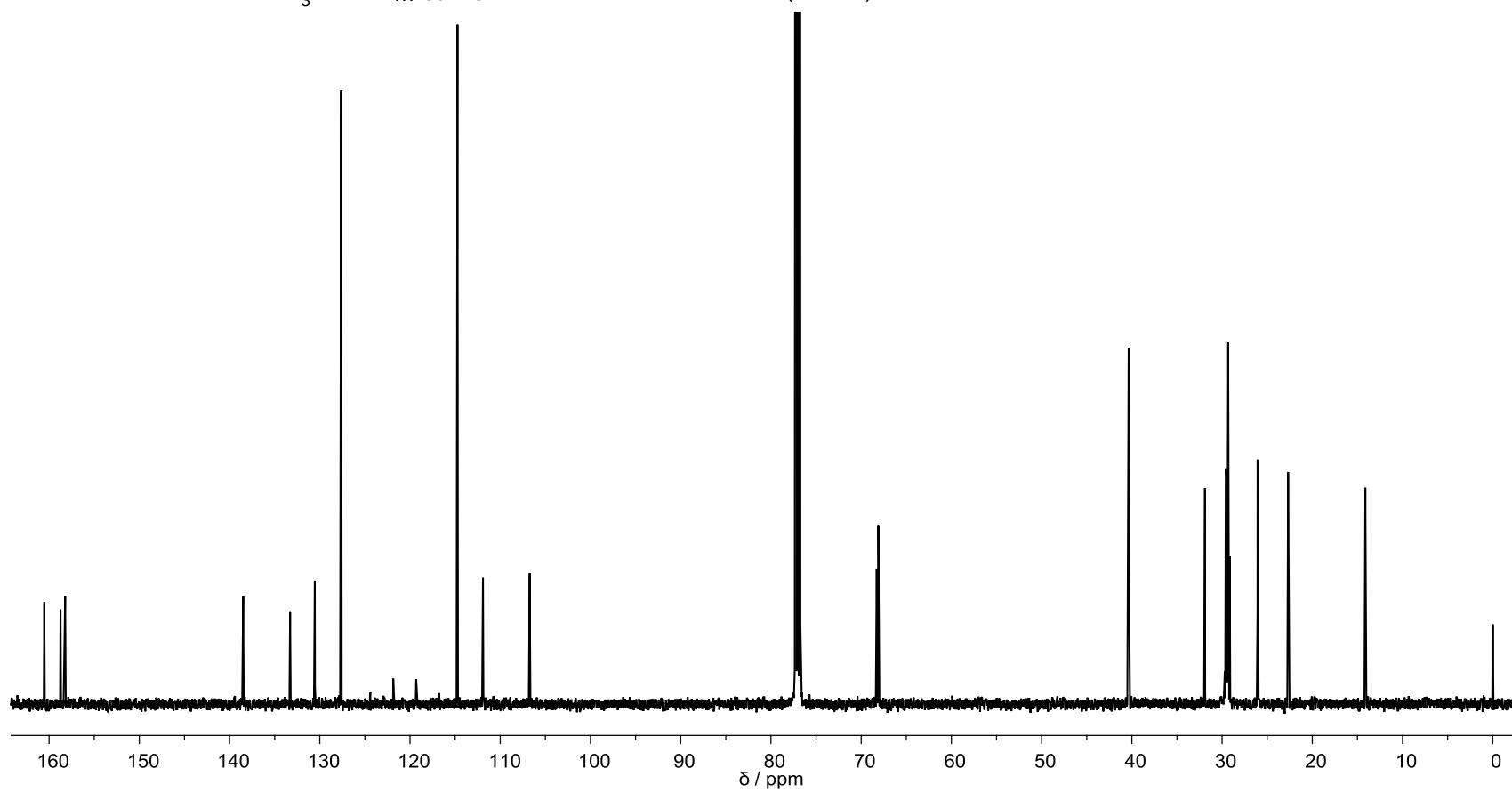
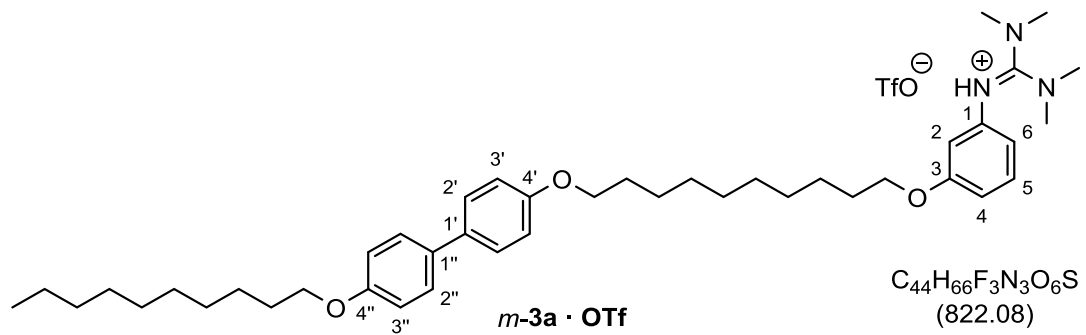
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste

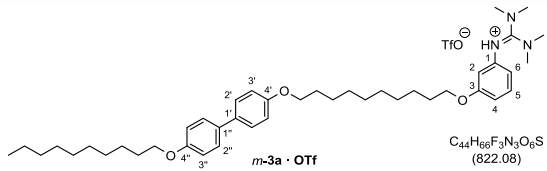








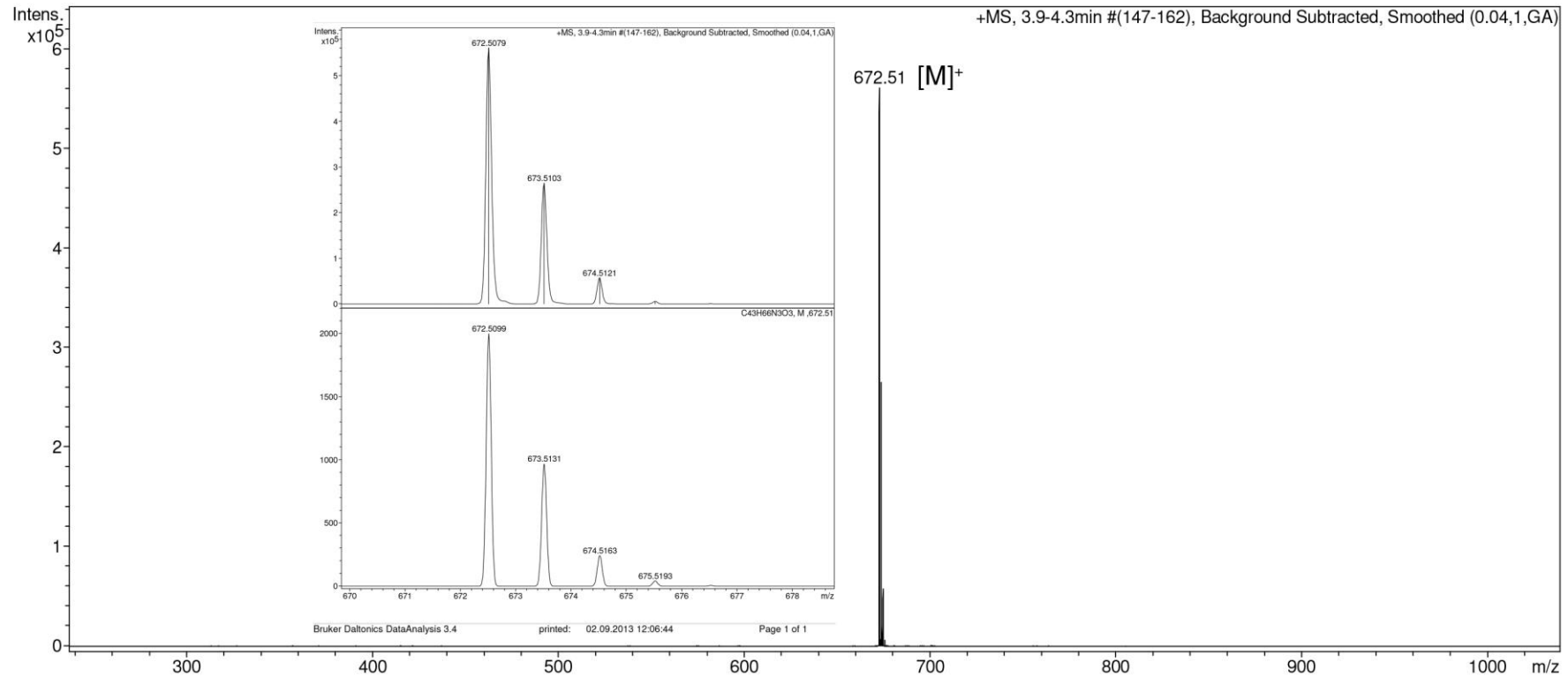
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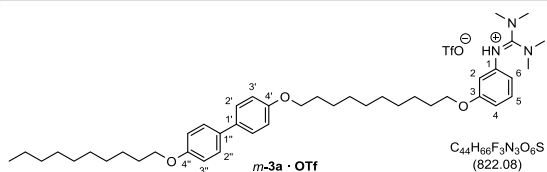
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 Operator wo/tri
 Instrument micrOTOF-Q 43

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	200 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste



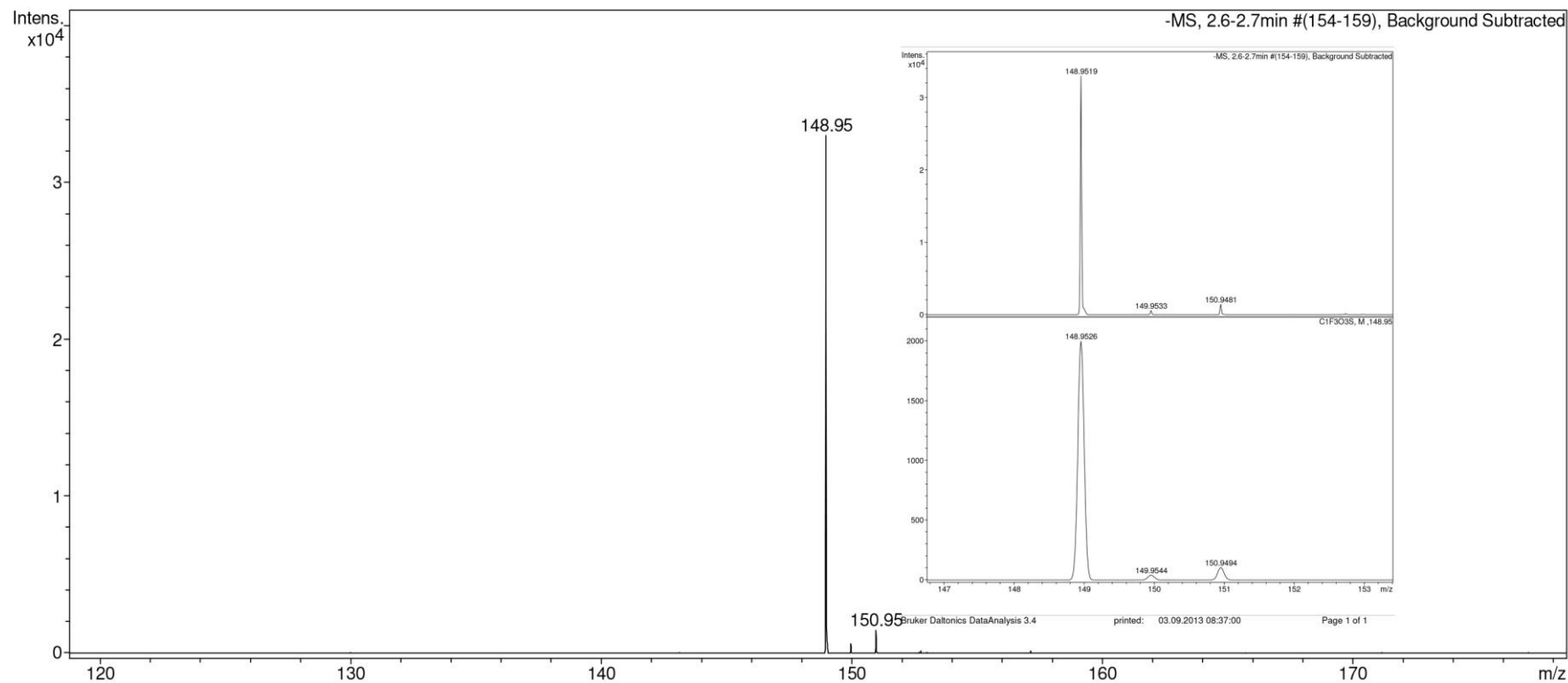
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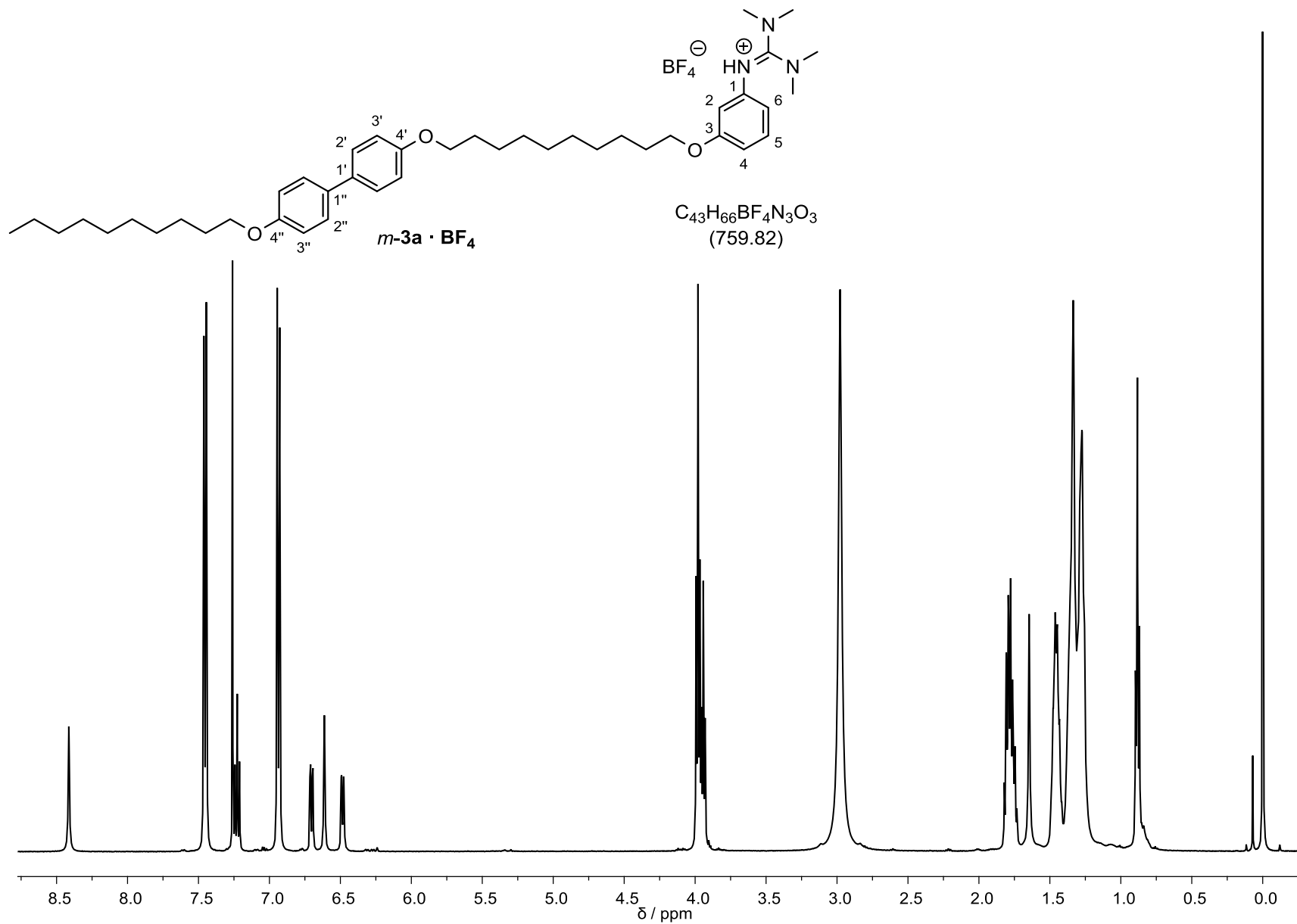


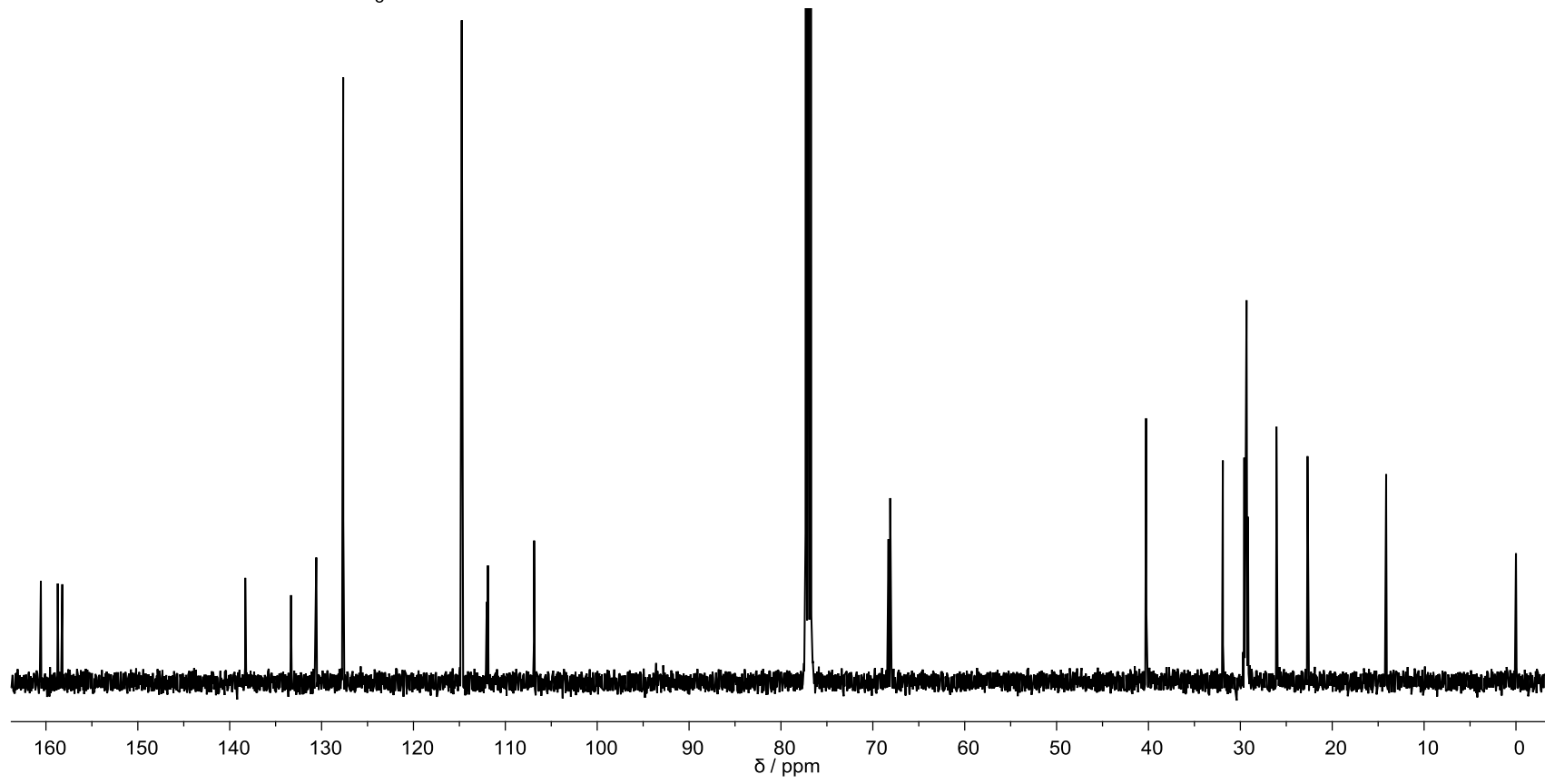
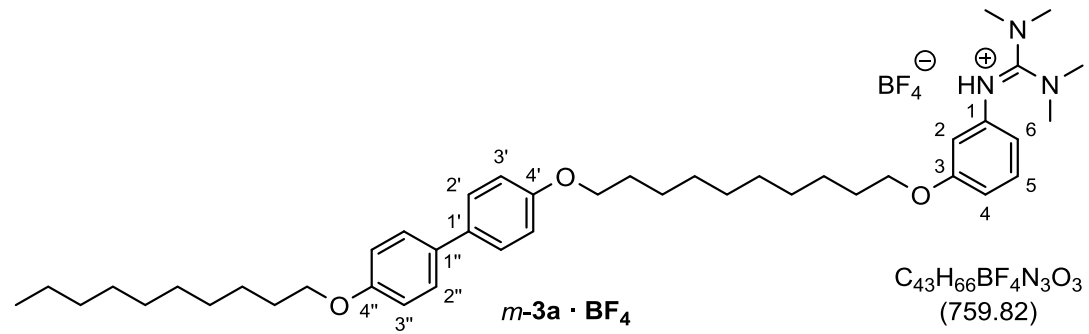
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 Operator wo/tri
 Instrument micrOTOF-Q 43

Acquisition Parameter

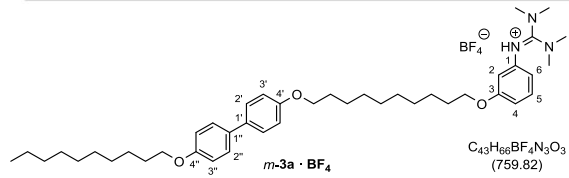
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Scan End	1000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste







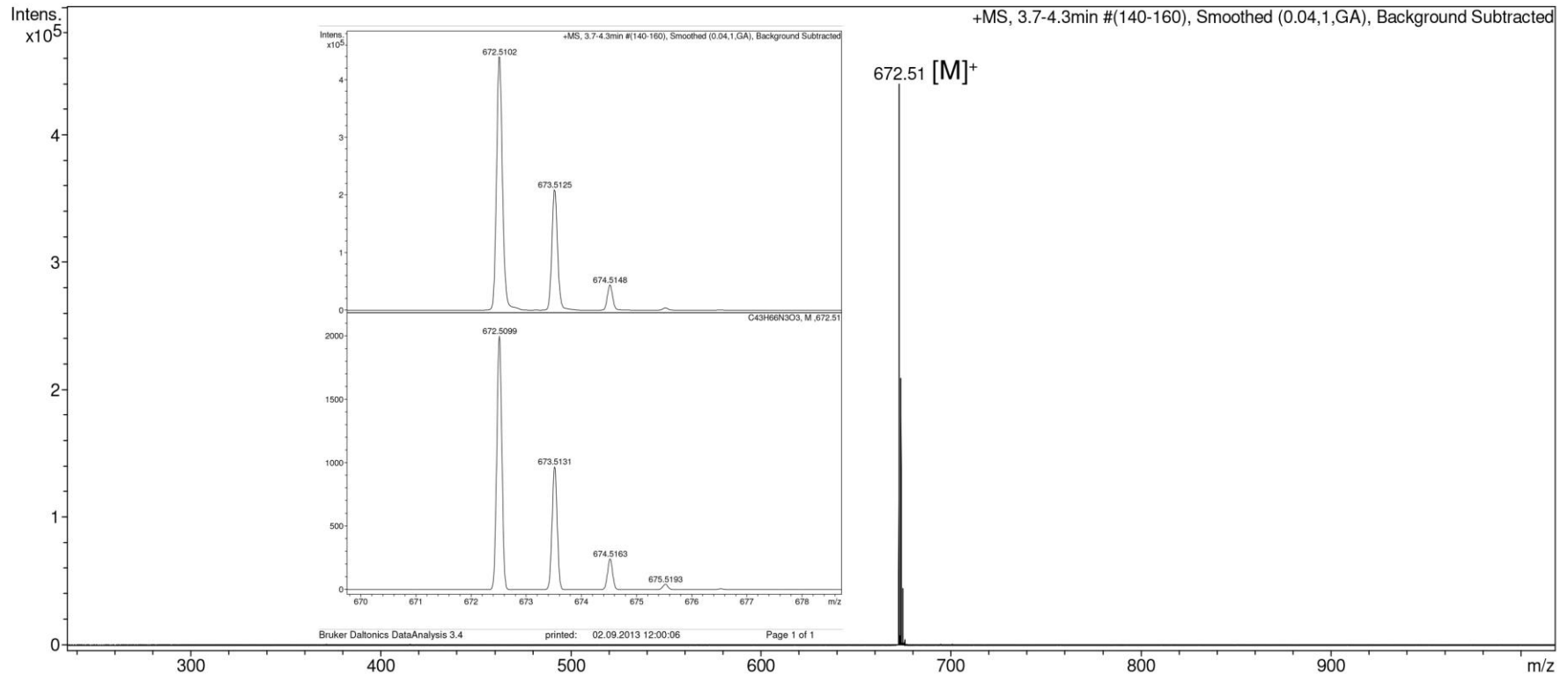
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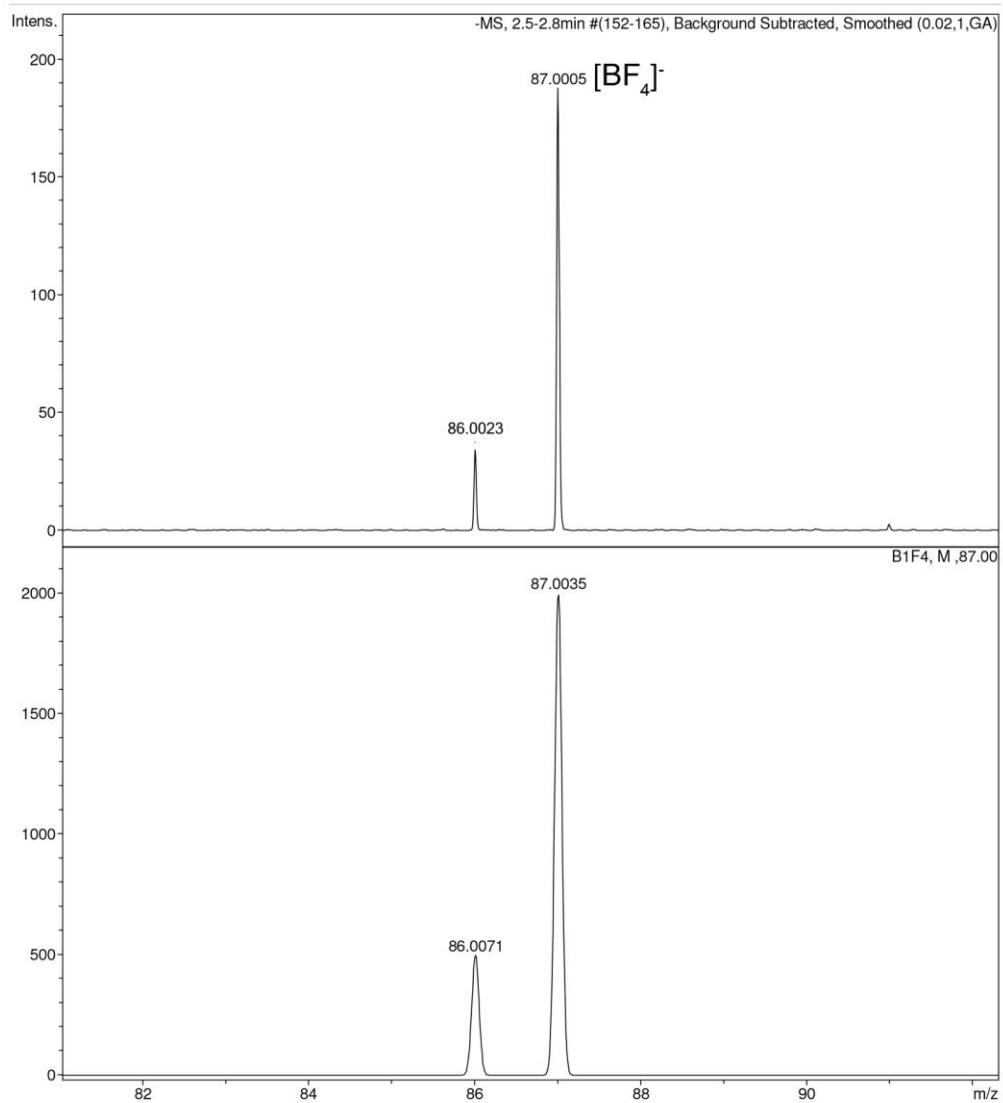
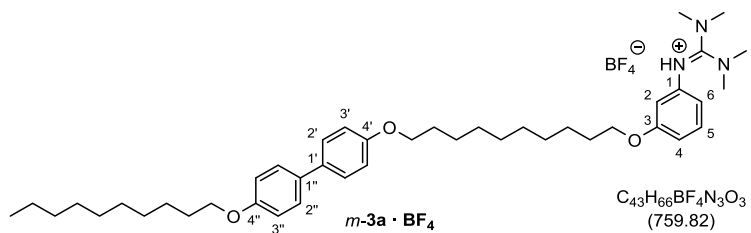


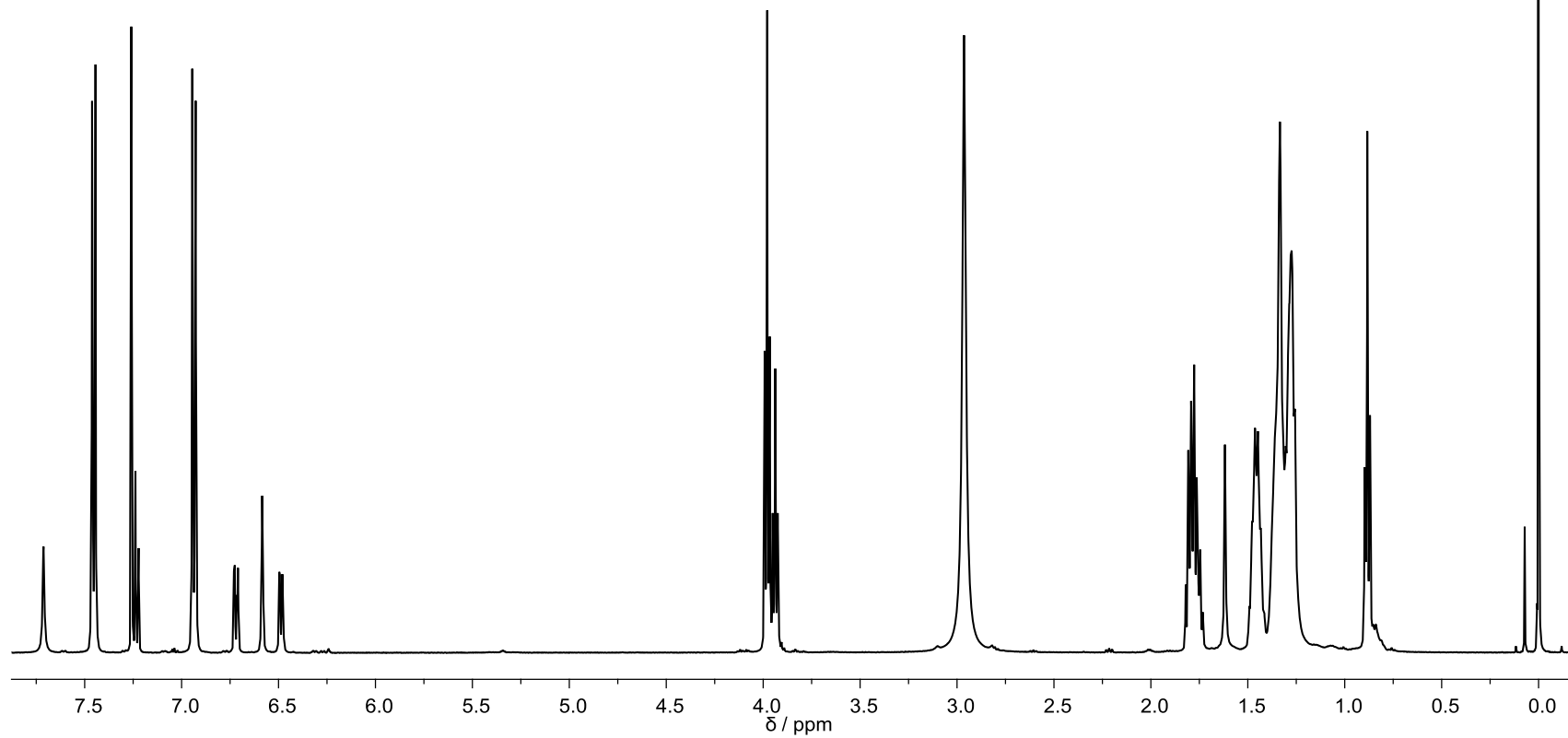
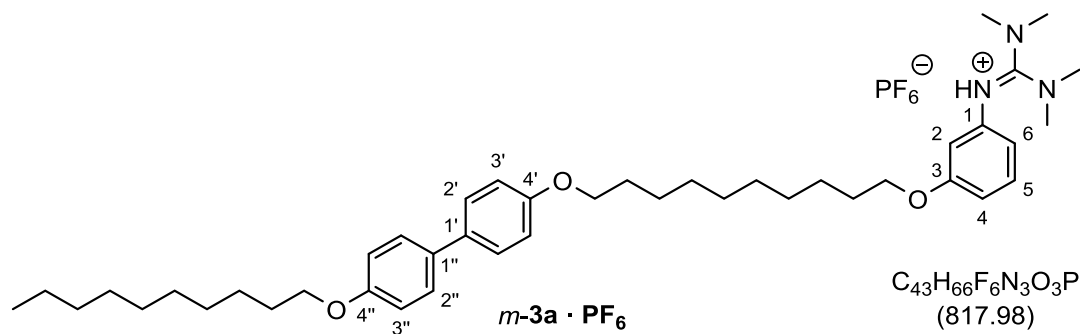
Acquisition Date 02.09.2013 11:12:24
Operator wo/tri
Instrument micrOTOF-Q 43

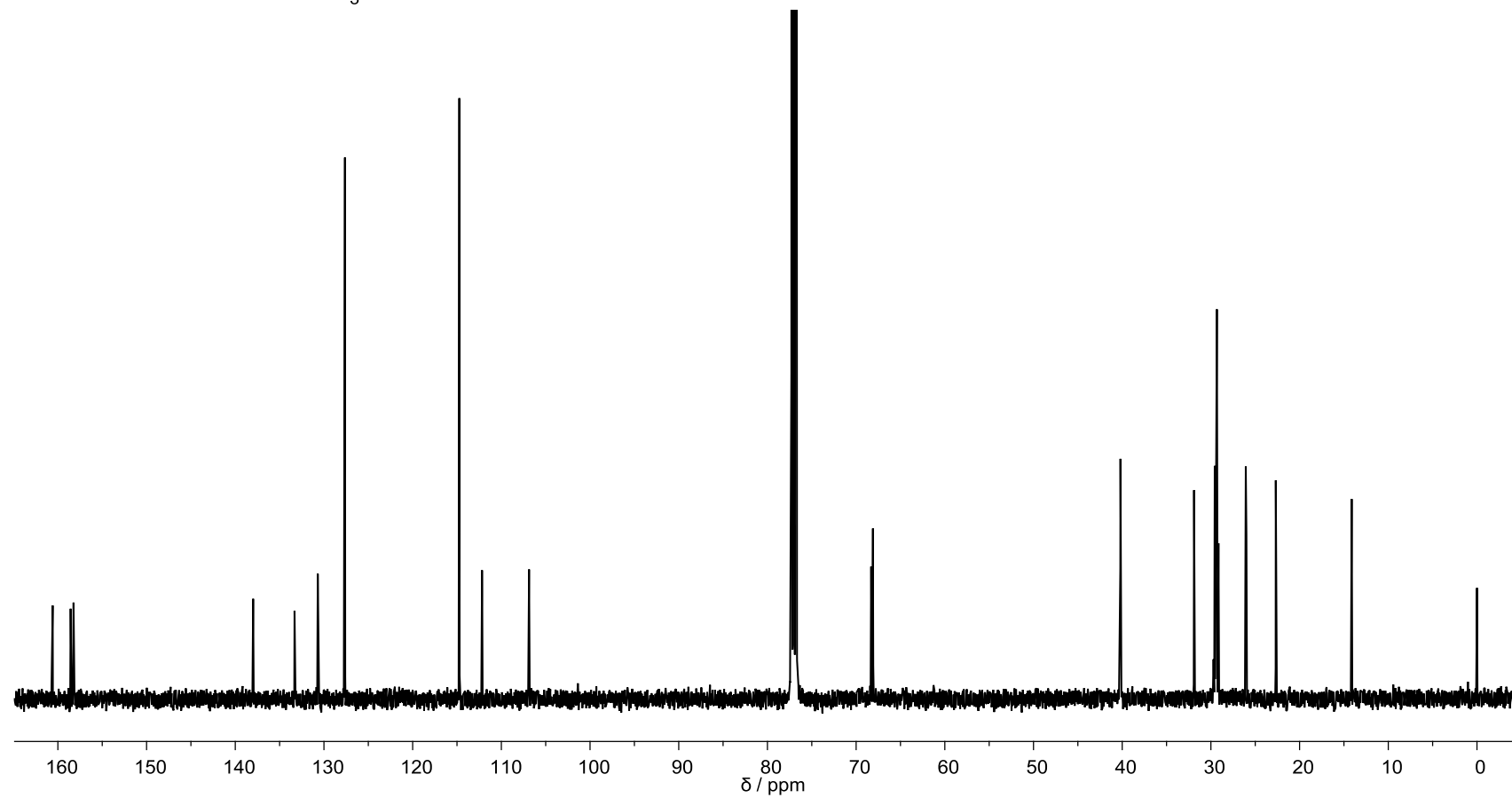
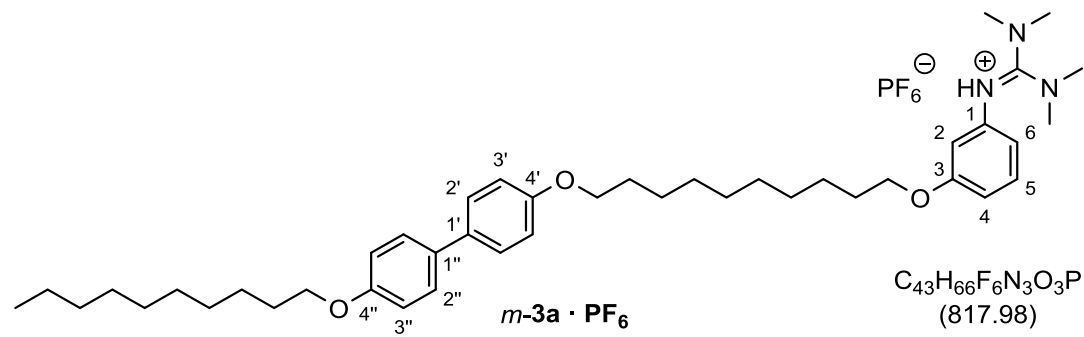
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Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
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Scan End	2500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste

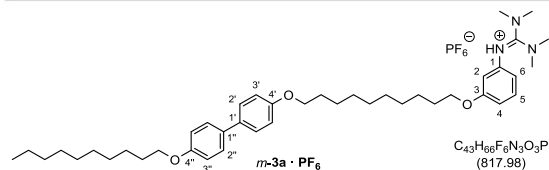








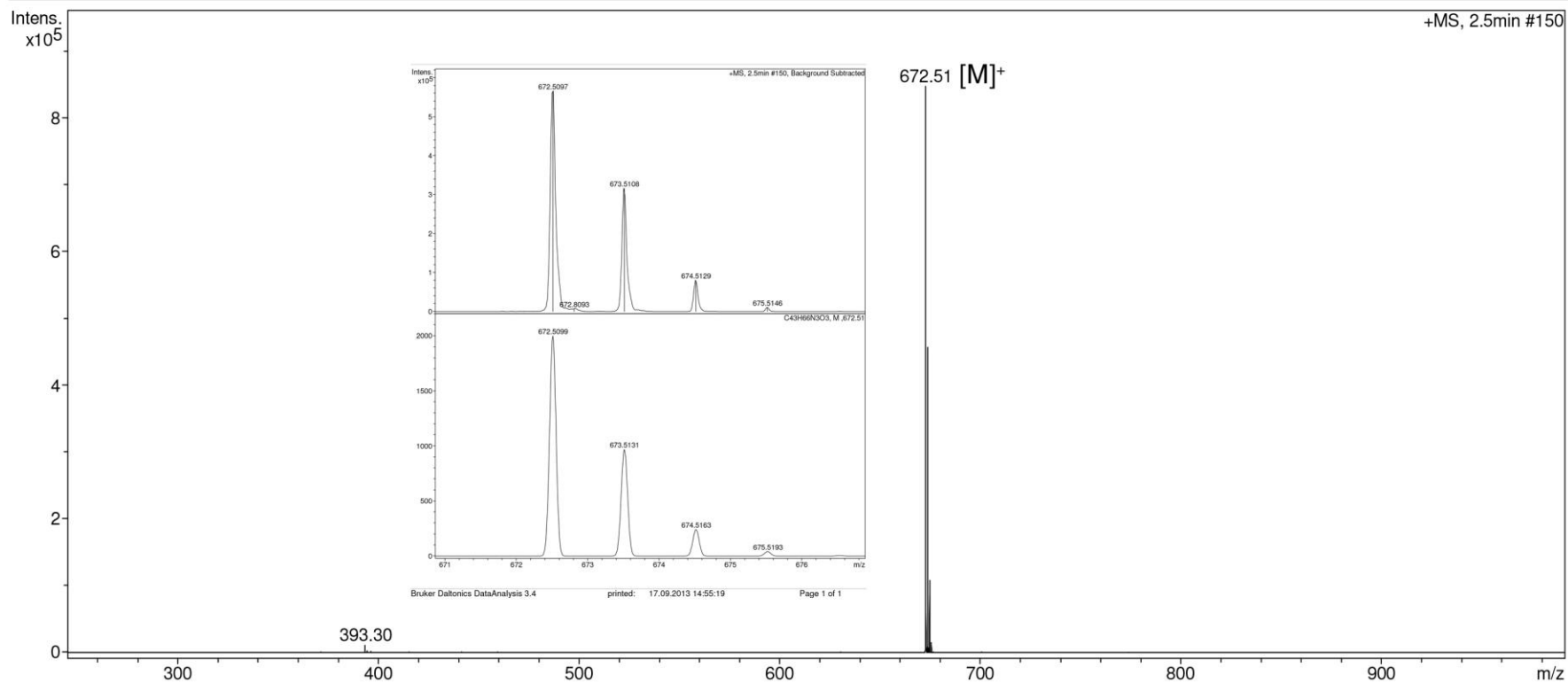
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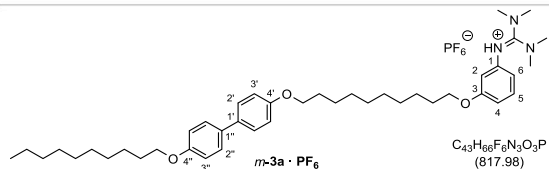
Acquisition Date 17.09.2013 11:59:35
 Operator wo/tri
 Instrument micrOTOF-Q 43

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	200 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste



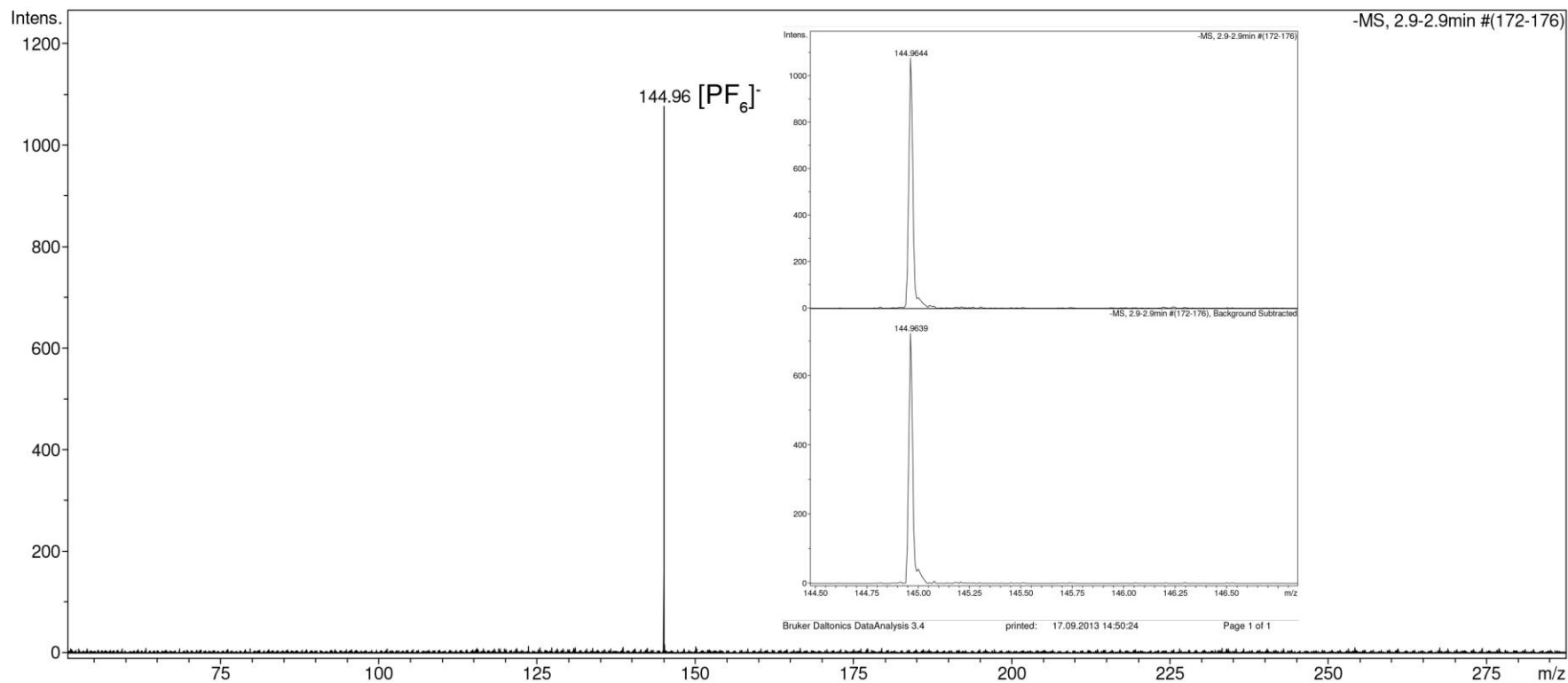
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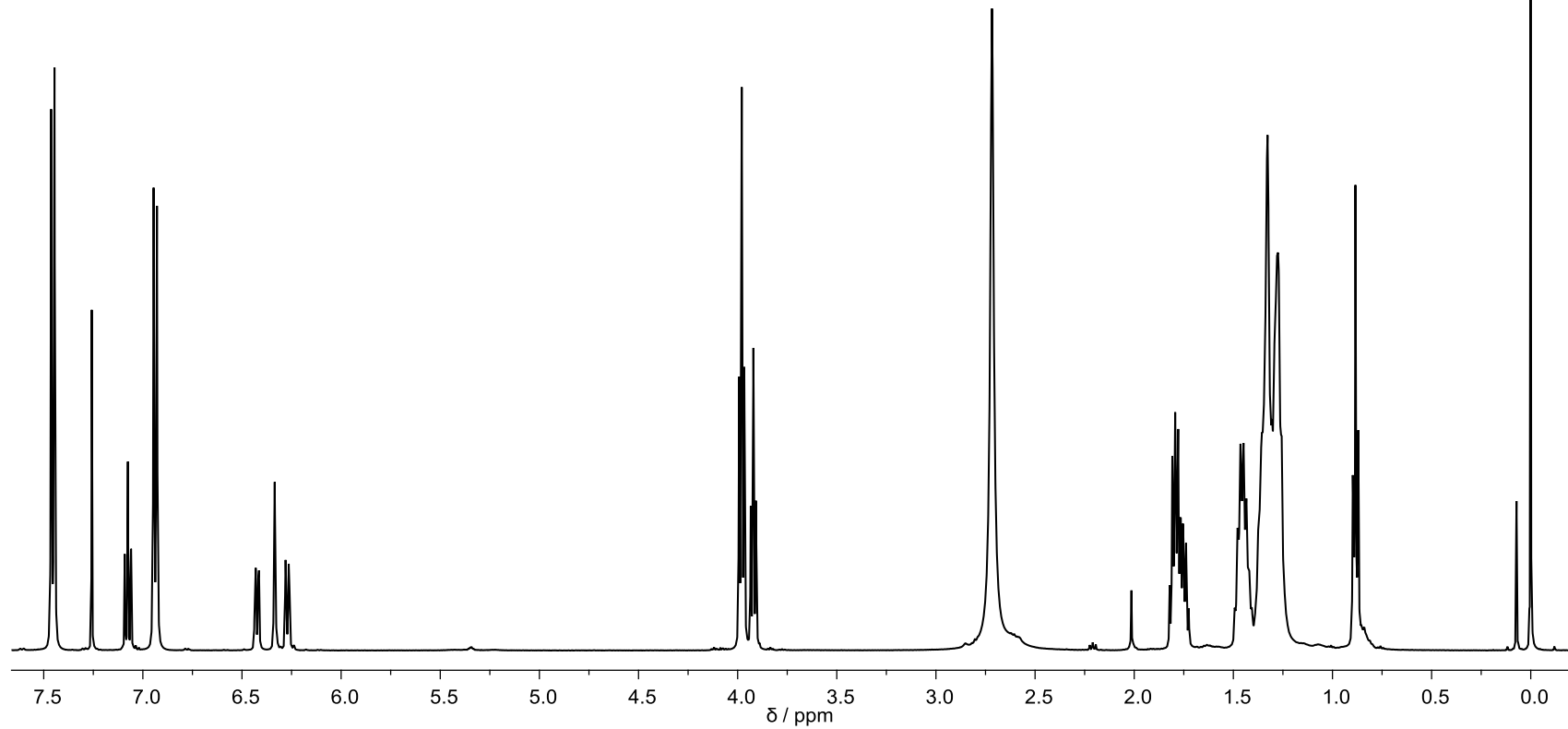
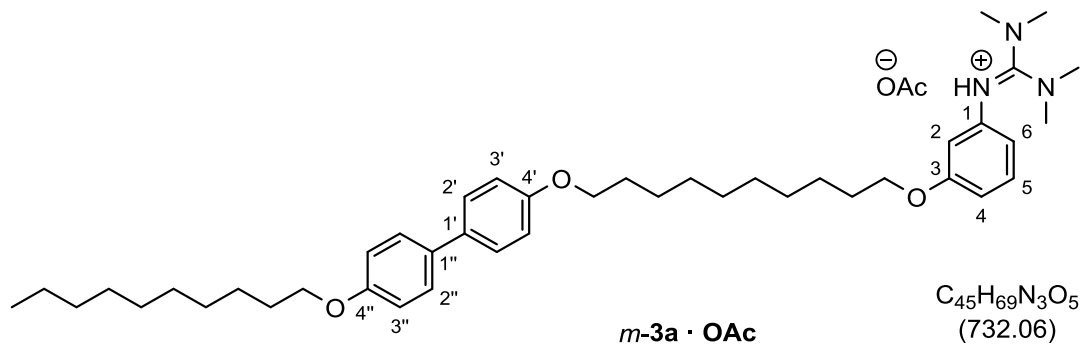


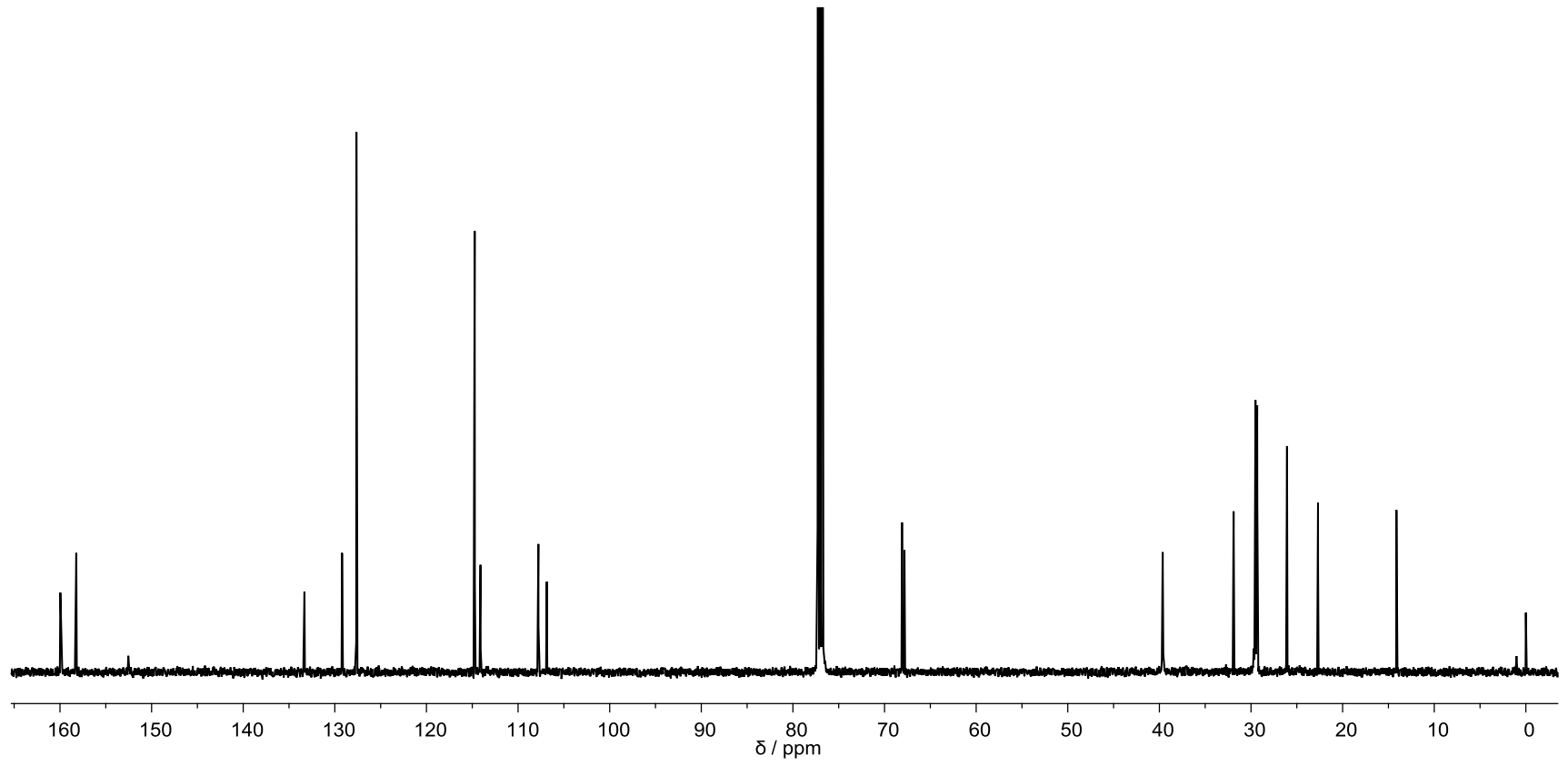
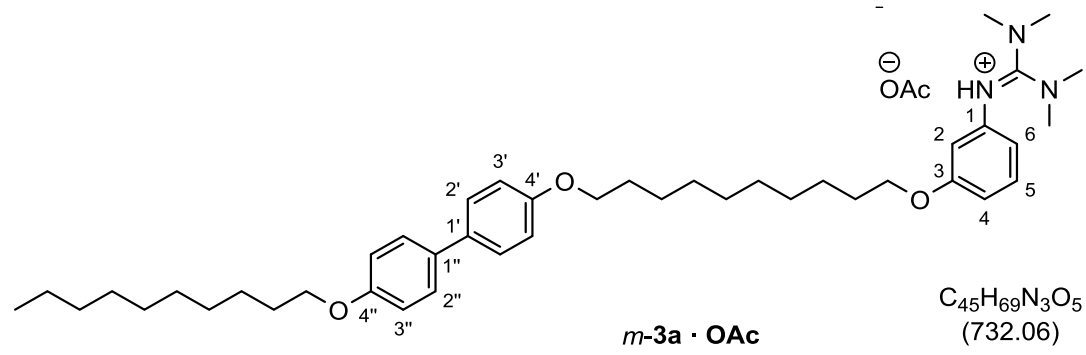
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 Operator wo/tri
 Instrument micrOTOF-Q 43

Acquisition Parameter

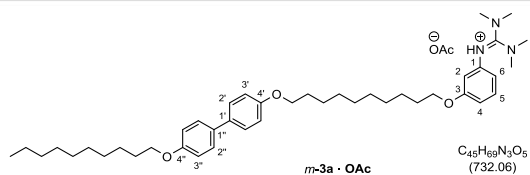
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Focus	Not active	Set Capillary	2000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste







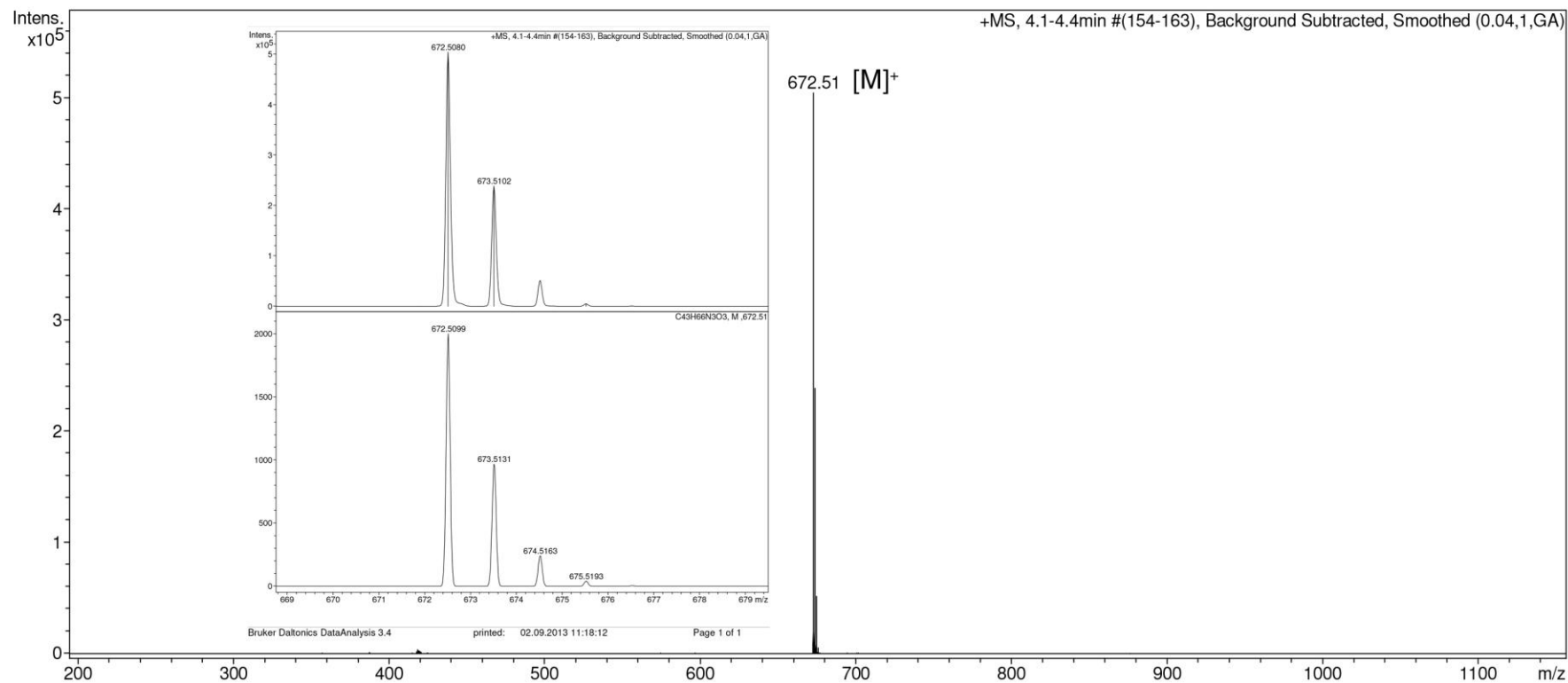
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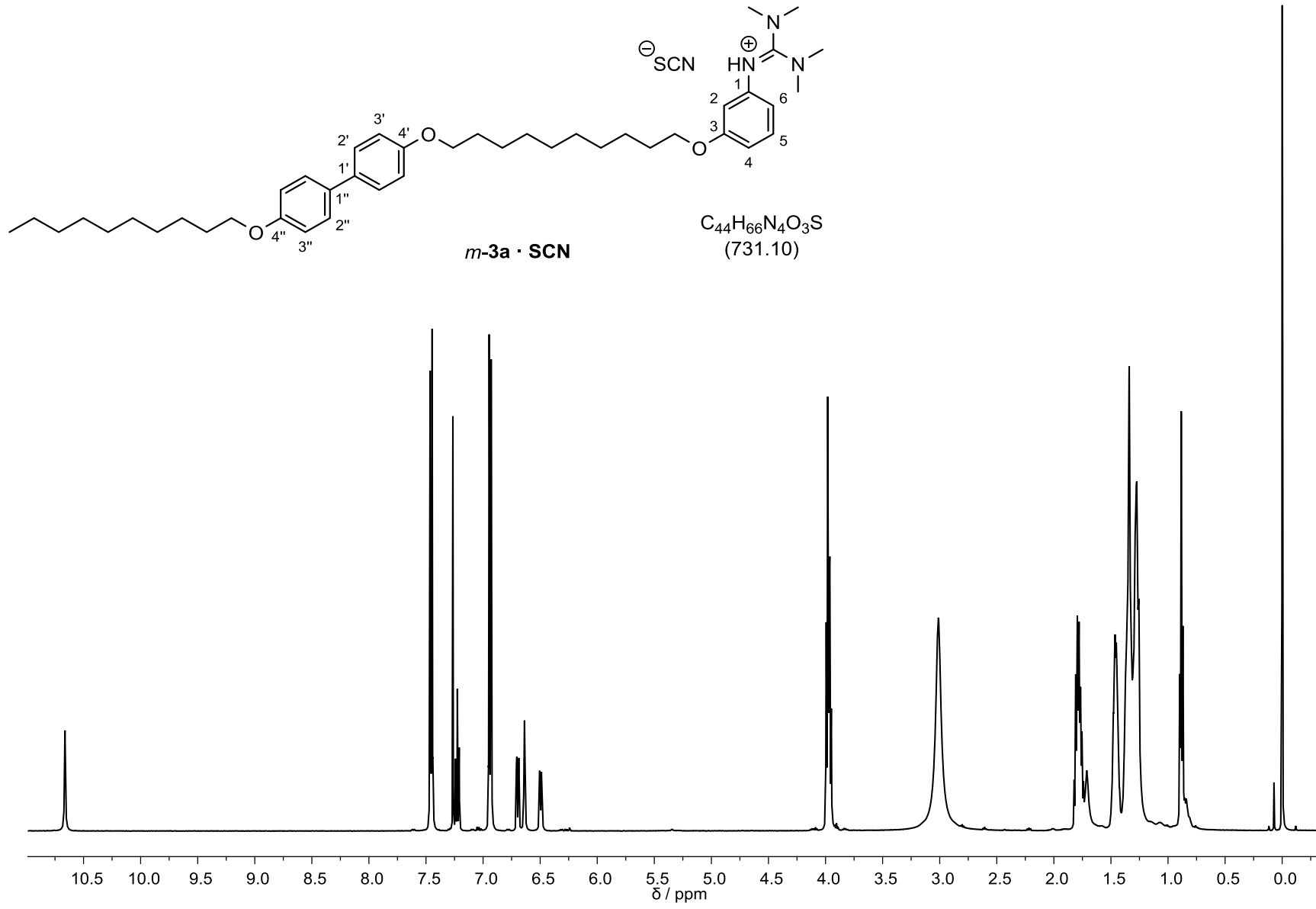


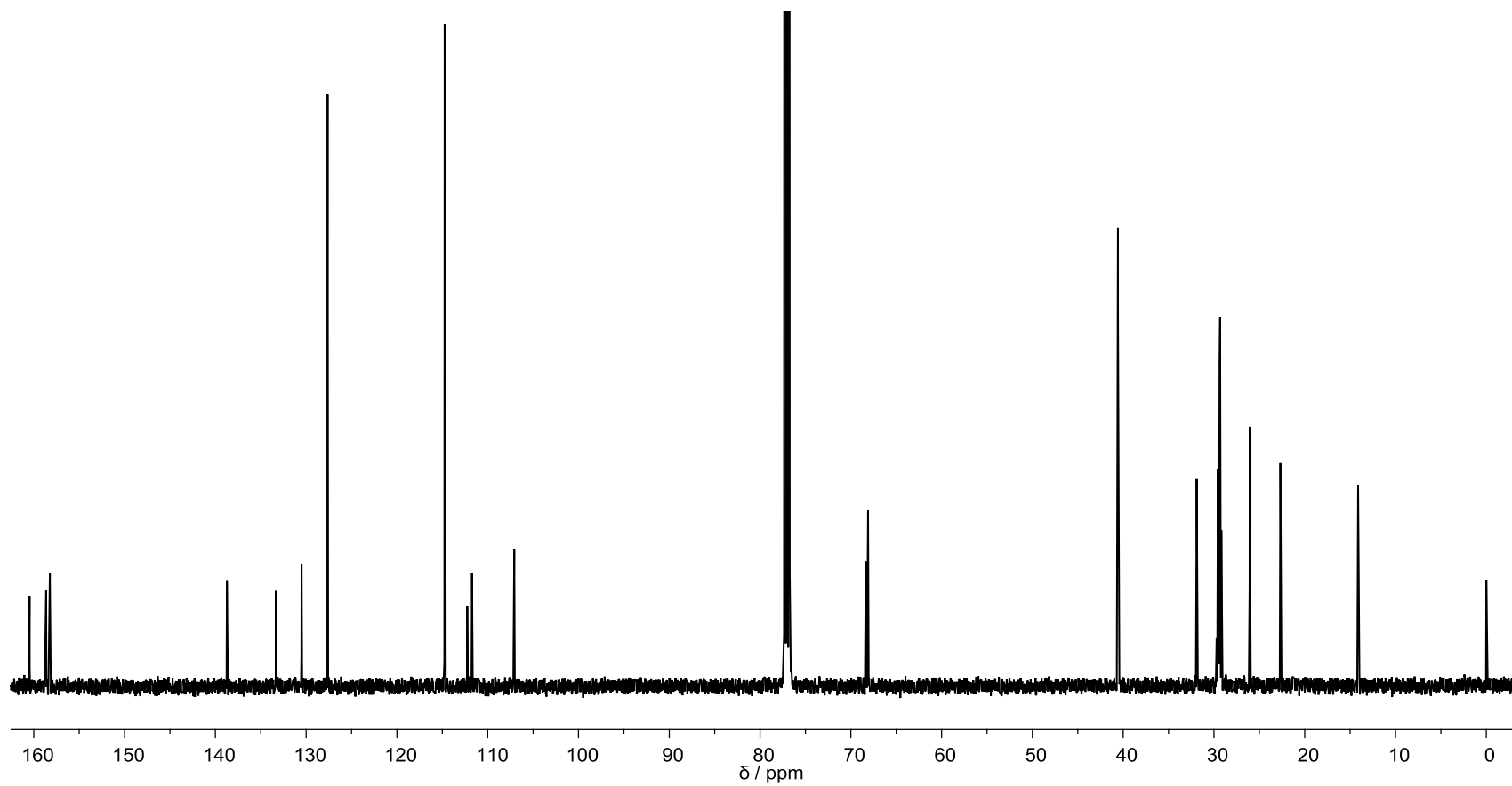
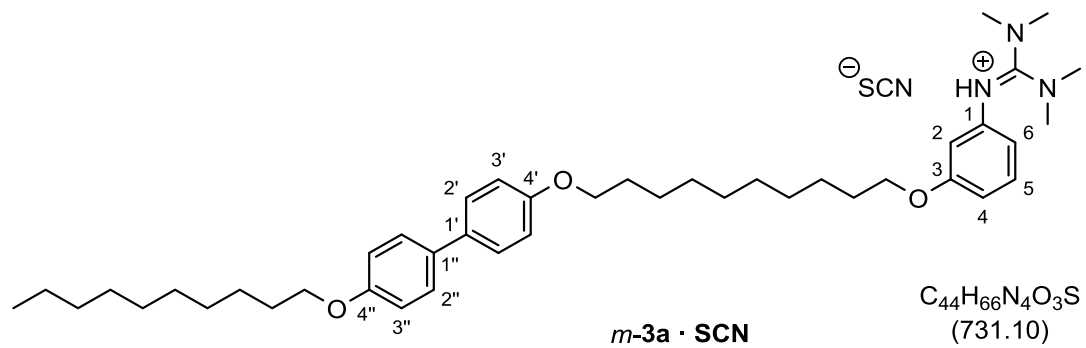
Acquisition Date 02.09.2013 11:04:03
 Operator wo/tri
 Instrument micrOTOF-Q 43

Acquisition Parameter

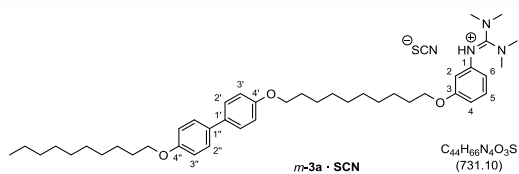
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Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	200 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste







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Acquisition Date 02.09.2013 11:41:21
Operator wo/tri
Instrument micrOTOF-Q 43

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	200 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste

