Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Photoresponsive ionic liquid crystals based on azobenzene guanidinium salts†

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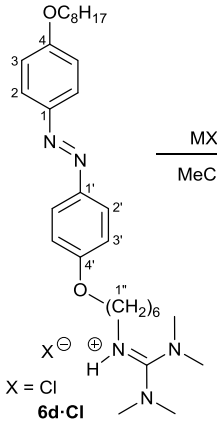
1) Synthesis of *N*-[6-(4-{(*E*)-[4-(octyloxy)phenyl]diazenyl}phenoxy)hexyl]tetramethylguanidinium salts (6d·X)



6d·X	yield [%]
6d·Br	86
6d·I	95
6d·OTf	89
6d·SCN	88
6d·PF_6	90
6d·BF_4	88

General procedure for the preparation of *N*-[6-(4-{(*E*)-[4-(octyloxy)phenyl]diazenyl}-phenoxy)hexyl]tetramethylguanidinium salts (6d·X) via salt metathesis. A solution of **6d·Cl** (34 μmol) in acetonitrile (5 mL) was treated with the respective salt (140 μmol) and the mixture was heated at 90 °C for 1 h and then cooled to r.t., while stirring was continued for 15 h. The solvent was removed *in vacuo* and the residue was dissolved in CH_2Cl_2, filtered over a syringe filter and concentrated.

Guanidinium bromide 6d·Br. Yellow solid (26 mg, 43 μmol, 86%). FT-IR (ATR): $\tilde{\nu}$ /cm^{-1} 2930s, 2854s, 1620s, 1599vs, 1579vs, 1496m, 1469m, 1404m, 1317m, 1297w, 1239vs, 1185w, 1147s, 1106m, 1071w, 1045w, 1023m, 996m, 945w, 898w, 848s, 836s, 814w, 778w, 761w, 731m, 720m, 639w, 553s. ^{1}H-NMR (250 MHz, $CDCl_3$): δ = 0.89 (t, *J* = 6.8 Hz, 3H, CH_3), 1.26–1.58 (m, 12H, CH_2), 1.76–1.87 (m, 8H, CH_2), 2.93 (br s, 6H, $N[CH_3]_2$), 3.09 (br s, 6H, $N[CH_3]_2$), 3.17–3.25 (m, 2H, NCH_2), 4.00–4.05 (m, 4H, 1''-H, OCH_2), 6.95–7.00 (m, 4H, 3,3'-H), 7.84–7.87 (m, 4H, 4,4'-H), 9.67 (br t, 1H, N-H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ = 14.1 (CH_3), 22.7, 25.6, 26.0, 26.6, 29.0, 29.2, 29.2, 29.4 29.7, 31.8 (CH_2), 39.9 ($N[CH_3]_2$), 40.6 ($N[CH_3]_2$),

45.4 (C-N), 67.9 (C-1''), 68.3 (C-O), 114.6 (C-3'), 114.7 (C-3), 124.3 (C-2',2), 146.9 (C-1'), 146.9 (C-1), 161.0 (C=N), 161.2 (C-4'), 161.4 (C-4) ppm. MS (ESI): *m/z* 524.40 $[M]^+$. HRMS (ESI): calcd. for $[C_{31}H_{50}N_5O_2]^+$ 524.3959, found 524.3967 $[M]^+$.

Guanidinium iodide 6d·I. Yellow solid (18 mg, 28 μmol, 95%). FT-IR (ATR): $\tilde{\nu}$ /cm^{-1} 3210m (br), 3177m, 3071w, 2922s, 2854s, 1616s, 1595vs, 1576vs, 1496s, 1468m, 1436w, 1410w, 1392m, 1314m, 1296m, 1238vs, 1184w, 1146vs, 1106m, 1064w, 1047w, 1020w, 1001w, 961w, 929w, 895w, 842vs, 813w, 783w, 754w, 731w, 677w, 639w, 573w. ^{1}H-NMR (250 MHz, $CDCl_3$): δ = 0.89 (t, *J* = 6.8 Hz, 3H, CH_3), 1.26–1.59 (m, 12H, CH_2), 1.76–1.88 (m, 8H, CH_2), 2.97 (br s, 6H, $N[CH_3]_2$), 3.10 (br s, 6H, $N[CH_3]_2$), 3.20–3.29 (m, 2H, NCH_2), 4.00–4.05 (m, 4H, 1''-H, OCH_2), 6.96–7.00 (m, 4H, 3,3'-H), 7.84–7.93 (m, 5H, 2,2'-H, NH) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ = 14.1 (CH_3), 22.7, 25.6, 26.0, 26.5, 29.0, 29.2, 29.2, 29.4 29.9, 31.0, 31.8 (CH_2), 40.3 ($N[CH_3]_2$), 41.1 ($N[CH_3]_2$), 45.1 (C-N), 67.9 (C-1''), 68.3 (C-O), 114.7 (C-3',3), 124.3 (C-2',2), 146.8 (C-1'), 146.9 (C-1), 161.0 (C=N), 161.2 (C-4'), 161.2 (C-4) ppm. MS (ESI): *m/z* (%) = 524.39 $[M]^+$. MS (ESI, neg.): *m/z* 126.90 $[I]^-$. HRMS (ESI): calcd. for $[C_{31}H_{50}N_5O_2]^+$ 524.3959, found 524.3950 $[M]^+$. HRMS (ESI, neg.): calcd. for I^- 126.9039, found 126.9045 $[I]^-$.

Guanidinium triflate 6d·OTf. Yellow solid (25 mg, 37 μmol, 89%). FT-IR (ATR): $\tilde{\nu}$ /cm^{-1} 2948m, 2922m, 2852m, 1621m, 1599s, 1578s, 1500m, 1471m, 1405w, 1317w, 1272s, 1245vs, 1142vs, 1107w, 1067w, 1030vs, 1004w, 970w, 943w, 903w, 839s, 809w, 778w, 756w, 733w, 637vs, 573m, 547s. ^{1}H-NMR (250 MHz, $CDCl_3$): δ = 0.89 (t, *J* = 6.8 Hz, 3H, CH_3), 1.26–1.58 (m, 14H, CH_2), 1.64–1.87 (m, 6H, CH_2), 2.95 (br s, 6H, $N[CH_3]_2$), 2.98 (br s, 6H, $N[CH_3]_2$), 3.13–3.21 (m, 2H, NCH_2), 4.00–4.05 (m, 4H, 1''-H, OCH_2), 6.95–7.00 (m, 4H, 3,3'-H), 7.84–7.87 (m, 5H, 2,2'-H, NH), 7.24 (br t, 1H, N-H) ppm. ^{13}C-NMR (125 MHz, $CDCl_3$): δ = 14.1 (CH_3), 22.7, 25.5, 26.0, 26.4, 28.9, 29.2, 29.2, 29.4 29.6, 31.0, 31.8 (CH_2), 39.9 ($N[CH_3]_2$), 45.4 (C-N), 67.9 (C-1''), 68.3 (C-O), 114.6 (C-3'), 114.7 (C-3), 118.1 (CF_3), 123.1 (CF_3), 124.3 (C-2',2), 146.8 (C-1'), 146.9 (C-1), 161.0 (C-4'), 161.2 (C-4), 161.6 (C=N) ppm. ^{1}H-NMR (250 MHz, CD_2Cl_2): δ = 0.89 (t, *J* = 6.8 Hz, 3H, CH_3), 1.30–1.89 (m, 20H, CH_2), 2.95 (br s, 12H, $N[CH_3]_2$), 3.15–3.26 (m, 2H, NCH_2), 4.01–4.07 (m, 4H, 1''-H, OCH_2), 6.98–7.01 (m, 4H, 3,3'-H), 7.17 (br s, 1H, N-H), 7.83–7.86 (m, 5H, 2,2'-H, NH) ppm. ^{13}C-NMR (63 MHz, CD_2Cl_2): δ = 14.3 (CH_3), 23.1, 26.0, 26.4, 26.8, 29.4, 29.6, 29.7, 29.8, 30.1, 32.2 (CH_2), 40.3 ($N[CH_3]_2$), 45.8 (C-N), 68.5 (C-1''), 68.8 (C-O), 115.0 (C-3',3), 124.6 (C-2',2), 147.2 (C-1'), 147.3 (C-1), 161.6 (C-4'), 161.8 (C-4), 162.1 (C=N) ppm. ^{19}F-NMR (235 MHz, $CDCl_3$): δ = –79.0 (s, CF_3) ppm. MS (ESI): *m/z* 524.40 $[M]^+$. MS (ESI, neg.): *m/z* 148.95 $[OTf]^-$. HRMS (ESI): calcd. for

$[C_{31}H_{50}N_5O_2]^+$ 524.3959, found 524.3966 $[M]^+$. HRMS (ESI, neg.): calcd. for Otf^- 148.9515, found 148.9517 $[M]^-$.

Guanidinium thiocyanate 6d·SCN. Yellow solid (23 mg, 39 μmol, 88%). FT-IR (ATR): $\tilde{\nu}$ / cm^{-1} 3149w (br), 3068w (br), 3041w, 2923s, 2854m, 2045vs (SCN^-), 1599s, 1579vs, 1497s, 1469s, 1406m, 1391w, 1366w, 1314m, 1294w, 1248vs, 1166w, 1140s, 1102m, 1064w, 1046w, 1024w, 1003m, 979w, 950w, 937w, 900w, 874w, 847s, 834vs, 805m, 778m, 745w, 728m, 689w, 640m, 594w, 559s, 548vs, 529w. ^{1}H-NMR (250 MHz, $CDCl_3$): δ = 0.89 (t, *J* = 6.8 Hz, 3H, CH_3), 1.26–1.59 (m, 12H, CH_2), 1.69–1.86 (m, 8H, CH_2), 2.96 (br s, 6H, $N[CH_3]_2$), 3.06 (br s, 6H, $N[CH_3]_2$), 3.14–3.22 (m, 2H, NCH_2), 4.00–4.06 (m, 4H, 1''-H, OCH_2), 6.96–7.00 (m, 4H, 3,3'-H), 7.84–7.89 (m, 4H, 2,2'-H), 8.33 (br t, 1H, N-H) ppm. ^{13}C-NMR (125 MHz, $CDCl_3$): δ = 14.1 (CH_3), 22.7, 25.6, 26.0, 26.5, 29.0, 29.2, 29.2, 29.4, 29.7, 31.8 (CH_2), 40.25 (br, $N[CH_3]_2$), 45.5 (C-N), 67.9 (C-1''), 68.3 (C-O), 114.7 (C-3',3), 124.3 (C-2',2), 146.9 (C-1'), 146.9 (C-1), 161.0 (C=N), 161.2 (C-4'), 161.5 (C-4) ppm. MS (ESI): *m/z* 524.40 $[M]^+$. HRMS (ESI): calcd. for $[C_{31}H_{50}N_5O_2]^+$ 524.3959, found 524.3966 $[M]^+$.

Guanidinium hexafluorophosphate 6d·PF_6. Yellow solid (27 mg, 40 μmol, 90%). FT-IR (ATR): $\tilde{\nu}$ /cm^{-1} 3394m, 2922s, 2868m, 2850m, 1599vs, 1578vs, 1499m, 1471m, 1424w, 1394m, 1322m, 1295w, 1237vs, 1186w, 1167w, 1142s, 1106m, 1026m, 1003w, 940w, 903w, 829vs, 777s, 726m, 663w, 641m, 557vs, 545s. ^{1}H-NMR (250 MHz, $CDCl_3$): δ = 0.89 (t, *J* = 6.8 Hz, 3H, CH_3), 1.26–1.57 (m, 12H, CH_2), 1.61–1.86 (m, 8H, CH_2), 2.95 (br s, 12H, $N[CH_3]_2$), 3.13–3.21 (m, 2H, NCH_2), 4.00–4.05 (m, 4H, 1''-H, OCH_2), 5.60 (t, *J* = 5.3 Hz, 1H, N-H), 6.95–6.99 (m, 4H, 3,3'-H), 7.83–7.87 (m, 4H, 2,2'-H) ppm. ^{13}C-NMR (125 MHz, $CDCl_3$): δ = 14.1 (CH_3), 22.7, 25.5, 26.0, 26.2, 26.2, 28.9, 29.2, 29.4, 29.7, 31.8 (CH_2), 39.7 (br, $N[CH_3]_2$), 45.5 (C-N), 67.9 (C-1''), 68.3 (C-O), 114.7 (C-3',3), 124.3 (C-2',2), 146.8 (C-1'), 146.9 (C-1), 161.0 (C=N), 161.2 (C-4'), 161.5 (C-4) ppm. MS (ESI): *m/z* 524.40 $[M]^+$. MS (ESI, neg.): *m/z* 144.96 $[PF_6]^-$. HRMS (ESI): calcd. for $[C_{31}H_{50}N_5O_2]^+$ 524.3959, found 524.3955 $[M]^+$. HRMS (ESI, neg.): calcd. for PF_6^- 144.9636, found 144.9643 $[M]^-$.

Guanidinium tetrafluoroborate 6d·BF_4. Yellow solid (21 mg, 32 μmol, 95%). FT-IR (ATR): $\tilde{\nu}$ /cm^{-1} 3353m, 2924s, 2854m, 1621s, 1596vs, 1577vs, 1497m, 1468m, 1420w, 1314m, 1297m, 1238vs, 1186w, 1147s, 1071s, 1033vs, 961w, 930w, 894w, 843vs, 812w, 784w, 757w, 639w, 574w, 553s. ^{1}H-NMR (250 MHz, $CDCl_3$): δ = 0.89 (t, *J* = 6.8 Hz, 3H, CH_3), 1.29–1.57 (m, 12H, CH_2), 1.68–1.87 (m, 8H, CH_2), 2.98 (br s, 12H, $N[CH_3]_2$), 3.14–3.22 (m, 2H, NCH_2), 4.00–4.05 (m, 4H, 1''-H, OCH_2), 6.48 (br t, 1H, N-H), 6.95–7.00 (m, 4H, 3,3'-H), 7.84–7.87 (m, 4H, 2,2'-H) ppm. ^{13}C-NMR (125 MHz, $CDCl_3$): δ = 14.1 (CH_3), 22.7, 25.6, 26.0, 26.3, 28.9, 29.2, 29.2, 29.4 29.6, 31.9 (CH_2), 39.9 ($N[CH_3]_2$), 45.5 (C-N), 67.9 (C-1''), 68.3 (C-O), 114.7 (C-3',3),

124.3 (C-2',2), 146.9 (C-1'), 146.9 (C-1), 161.0 (C=N), 161.2 (C-4'), 161.7 (C-4) ppm. MS (ESI): *m/z* (%) = 524.40 $[M]^+$. MS (ESI, neg.): *m/z* 87.00 $[M]^-$. HRMS (ESI): calcd. for $[C_{31}H_{50}N_5O_2]^+$ 524.3959, found 524.3952 $[M]^+$.

2) DSC measurements of guanidinium salts 6d·X

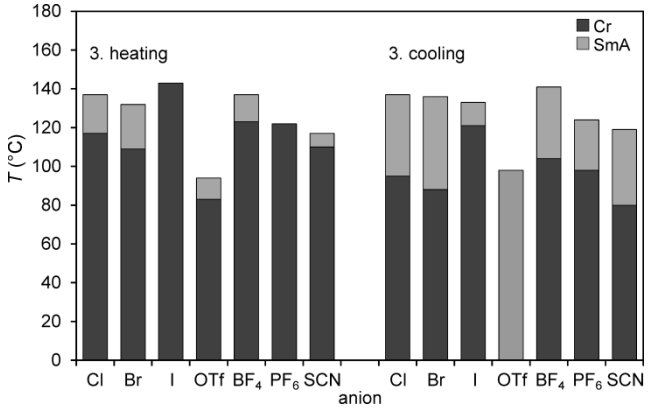


Fig. S1 Mesophase widths depending on the anion X (heating/cooling rate 10 K min^{-1}).

Table S1 Phase transition temperatures [°C] (and enthalpies [kJ mol^{-1}]) of guanidinium azobenzene ILCs **6d·X** upon third heating/cooling cycle[a,b]

Compd	Cr		SmA		I	Cycle
6d·Br	●	109 (28.6)	●	132 (1.4)	●	heating
	●	88 (24.7)	●	136 (1.6)	●	cooling
6d·I	●	143 (40.3)	–	–	●	heating
	●	121 (38.8)	●	133 (1.5)	●	cooling
6d·OTf	●	83 (29.2)	●	94 (5.8)	●	heating
	–	–	●	98 (4.7)	●	cooling
6d·BF_4	●	123 (34.1)	●	137 (1.4)	●	heating
	●	104 (32.7)	●	141 (1.7)	●	cooling
6d·PF_6	●	122 (38.0)	–	–	●	heating
	●	98 (32.6)	●	124 (1.8)	●	cooling
6d·SCN	●	110 (49.9)	●	117 (2.0)	●	heating
	●	80 (44.5)	●	119 (2.0)	●	cooling

[a] Heating/cooling rate 10 K min^{-1}. [b] The following phases were observed: crystalline (Cr), smectic A (SmA), isotropic (I).

3) Photoisomerization of 6c·Cl in ILC matrix (C_{12}MIMBr)

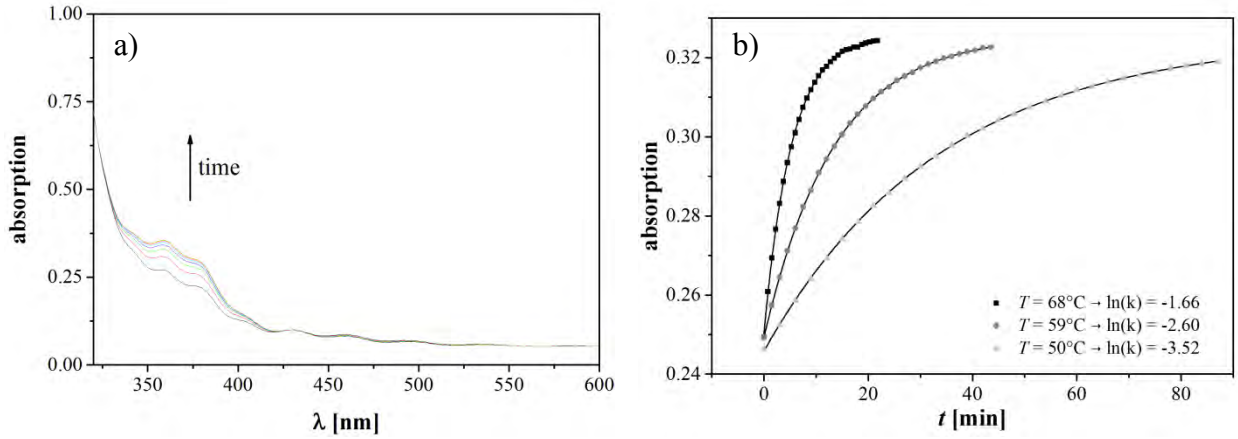


Fig. S2 Photoisomerization experiments of ILC **6c·Cl.** (a) Wavelength-dependent absorption spectra in the ILC matrix (C_{12}MIMBr) during E/Z-reisomerization at T = 68 °C. The regular fringes are due to reflections within the LC-cell. (b) UV-Vis absorption at 360 nm vs. time curves for **6c·Cl** in the ILC host (symbols) as well as the mono exponential fit curves (black solid lines) for different temperatures and the obtained rate constants.

4) Single-crystal X-ray structure analysis of guanidinium bromide 6b·Br and 6a·Cl

Guanidinium bromide **6b·Br**

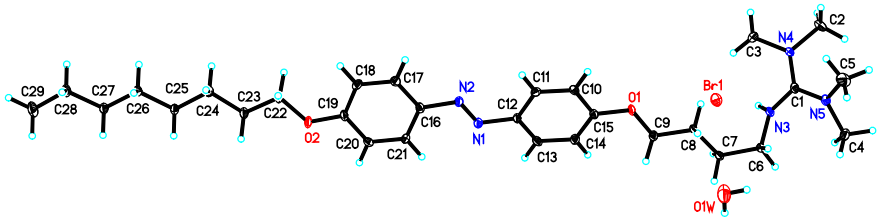


Table S2 Weak intermolecular electrostatic interaction in solid state

Donor-H	Acceptor (Acc.)	Symop. (Acc.)	Distance H–Acc. (Å)	Angle D-H–Acc. (°)
C13-H13	O2	1.0-x, -y, 1.0-z	2.71	169
C5-H5B	O1	3.0-x, -1.0-y, z	2.93	105
C26-H26B	N1	1.0-x, 1.0-y, 1.0-z	2.93	152
C27-H27A	N1	-x, 1.0-y, 1.0-z	2.89	151
C7-H7B	N2	1.0+x, -1.0+y, z	2.73	172
C4-H4A	N4	3.0-x, -2.0-y, -z	2.88	130
C4-H4B	Br1	1.0+x, y, z	2.80	149

Crystal structure determination of guanidinium chloride 6a·Cl (CCDC-1030120)

Crystal data. $C_{31}H_{48}Cl_7N_5O_2$, M = 770.89, monoclinic, a = 9.7566(5)(1), b = 9.1438(5), c = 42.575(2) Å, V = 3797.3(4) Å^3, T = 100 K, space group P 21/c, Z = 4, 27166 reflections measured, 6758 unique (R_{int} = 0.0439) which were used in all calculations. The final $wR(F_2)$ was 0.0827 (all data).

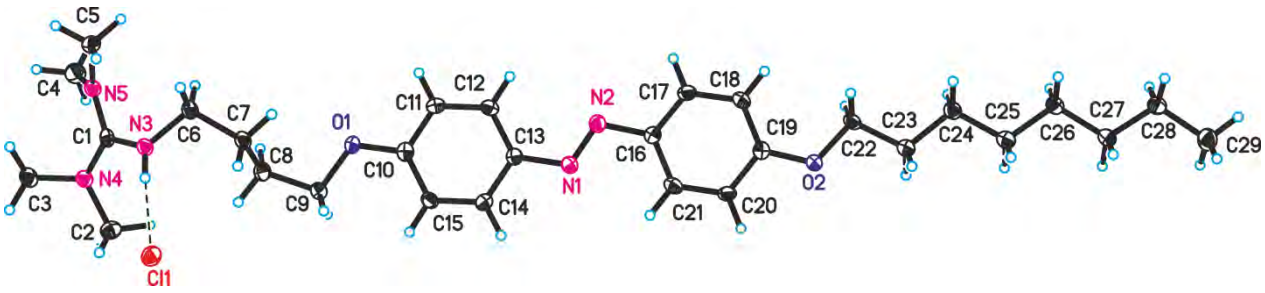


Fig. S3 X-ray structure of **6a·Cl** in the solid state.

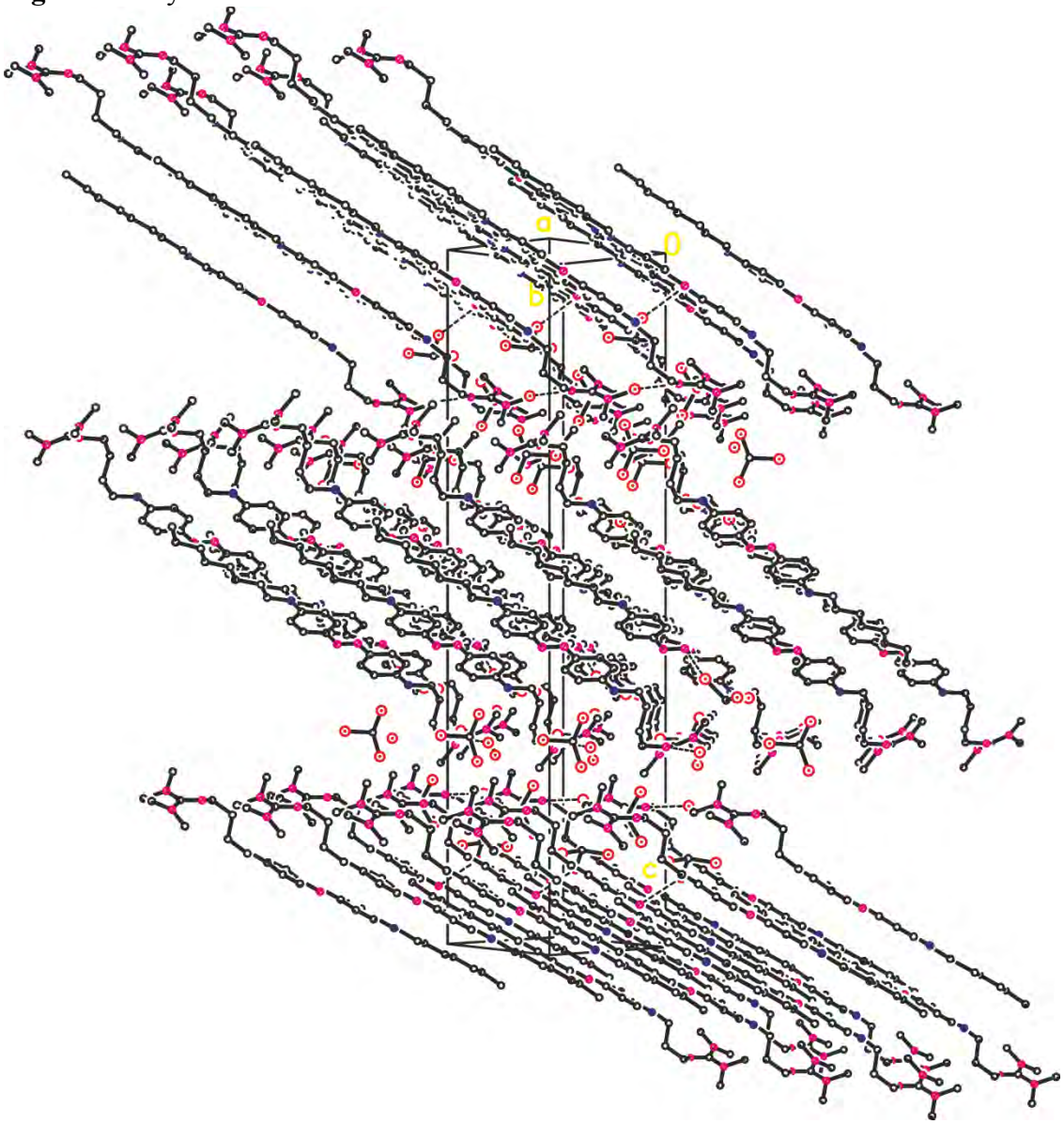
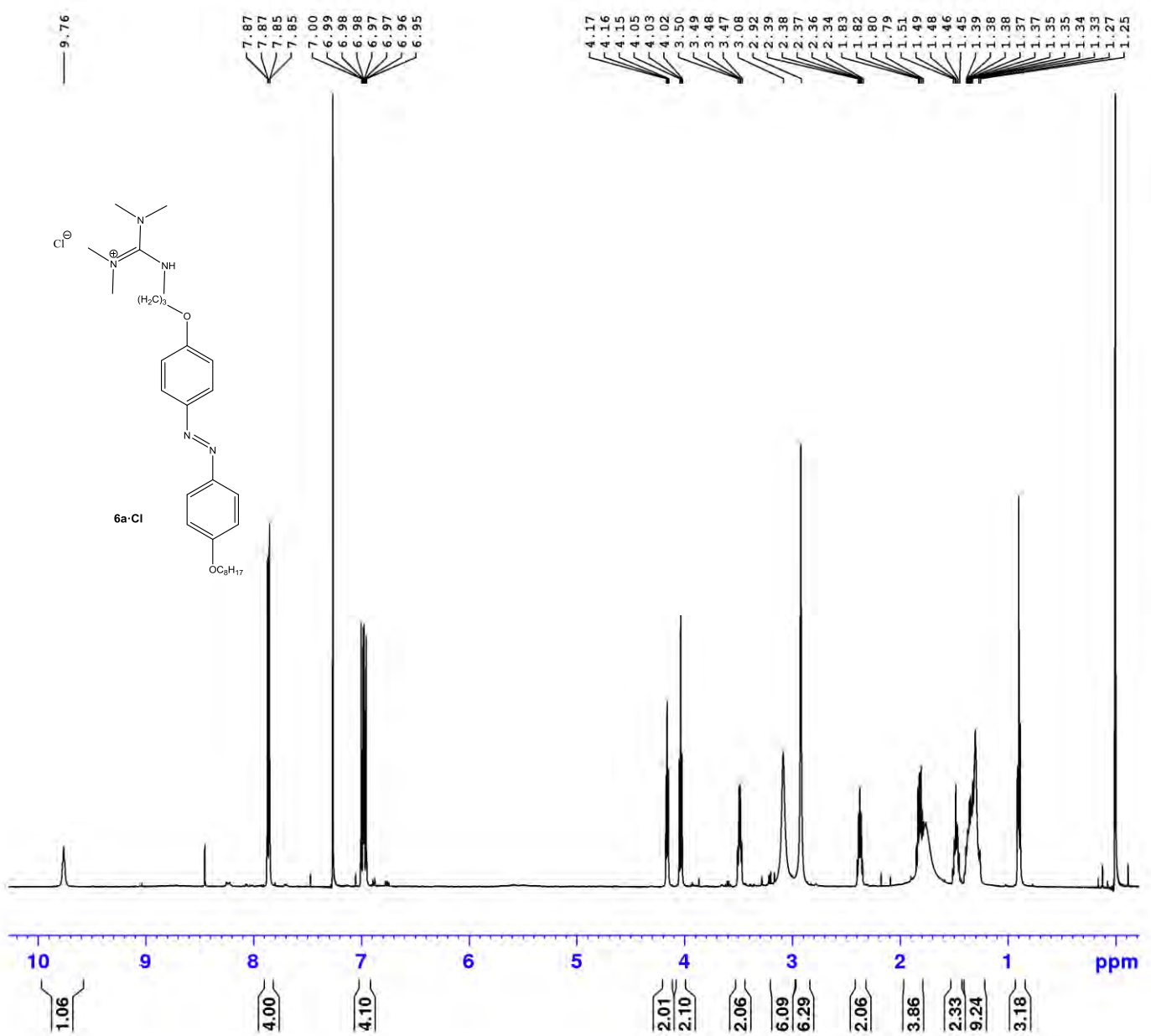


Fig. S4 Packing diagram for **6a·Cl**.

5) Data of azobenzene ILCs 6

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DE                        10.00 usec
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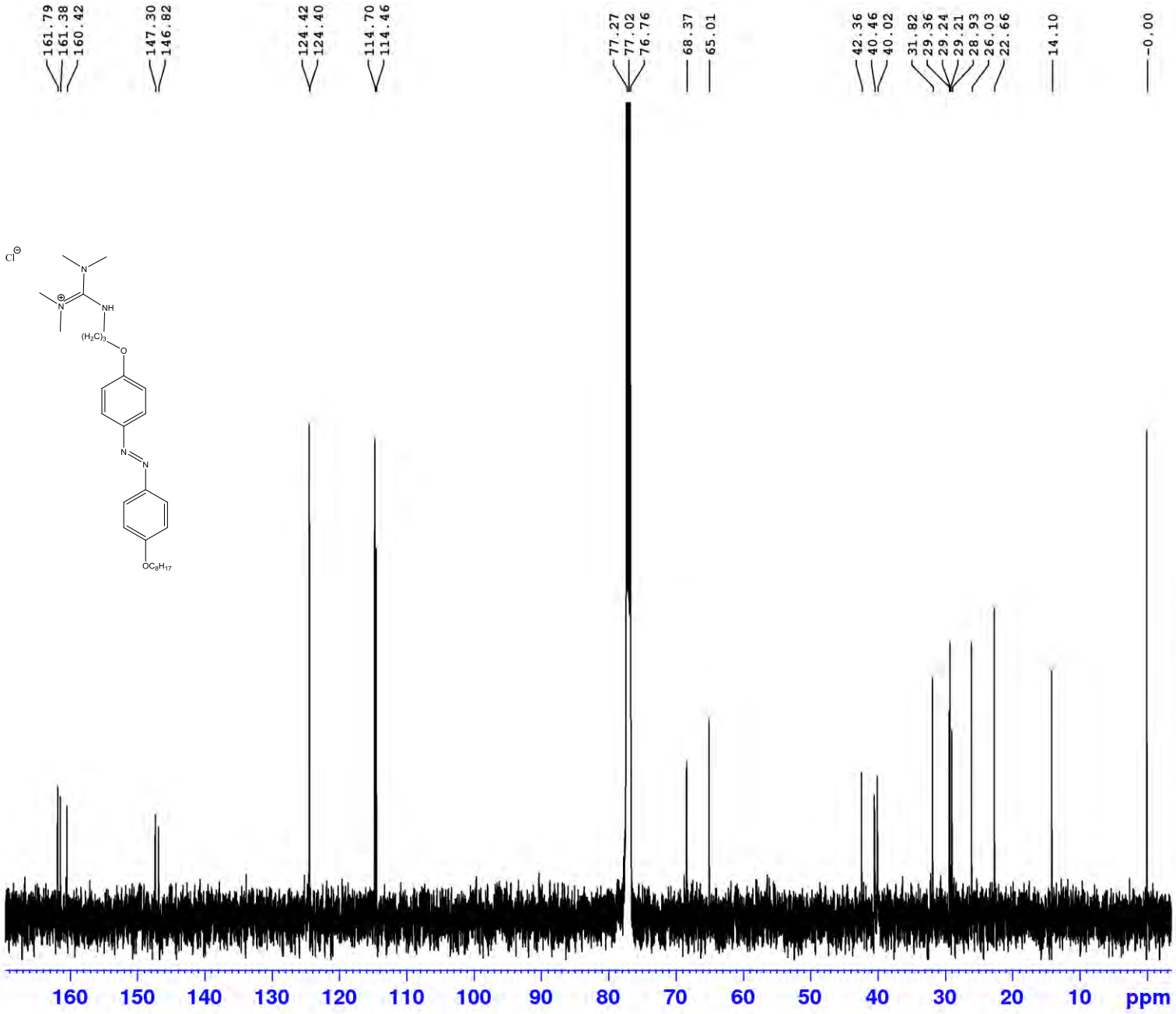

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TE 296.8 K
D1 2.00000000 sec
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PL12 19.99 dB
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^exo

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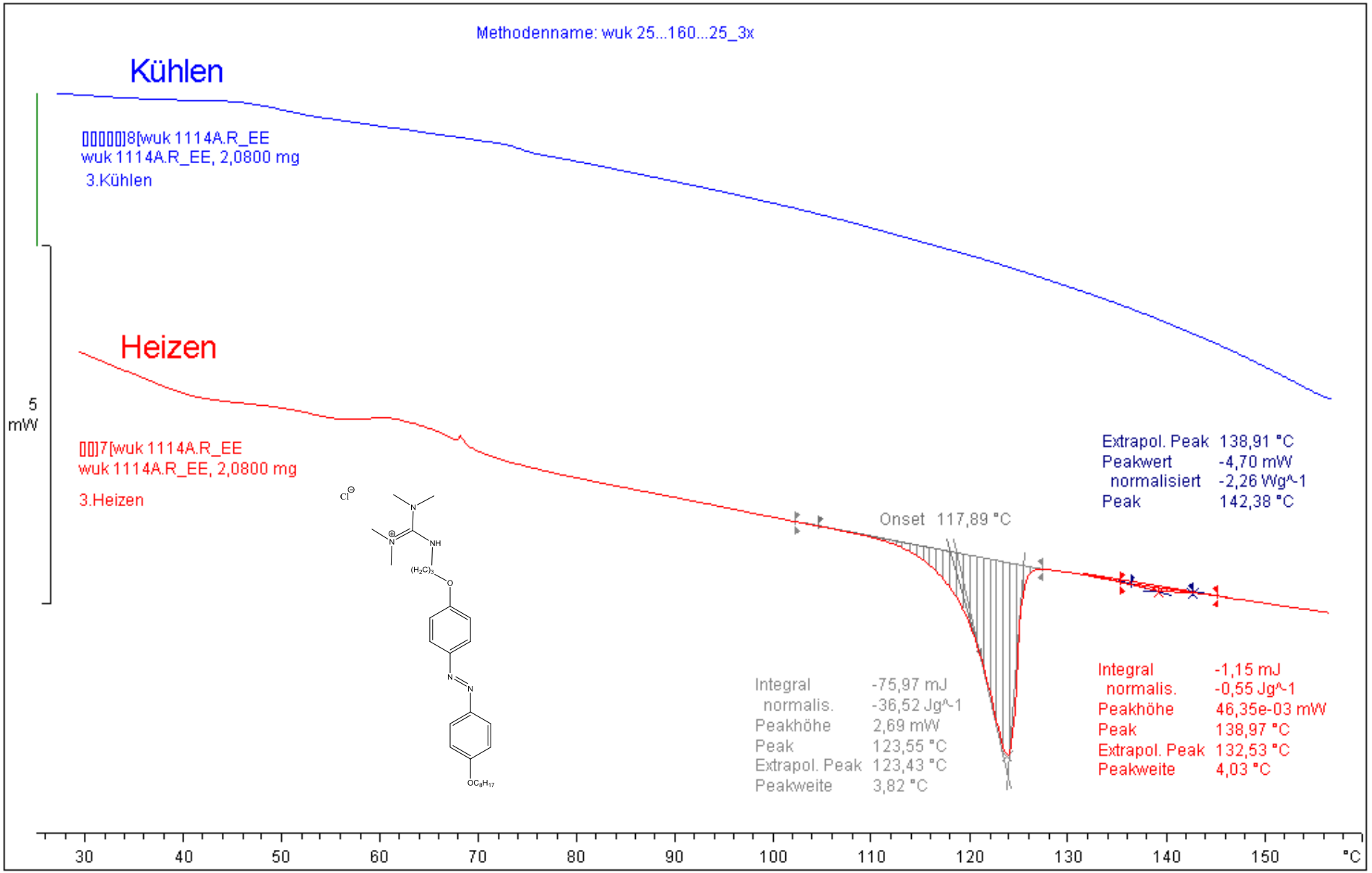

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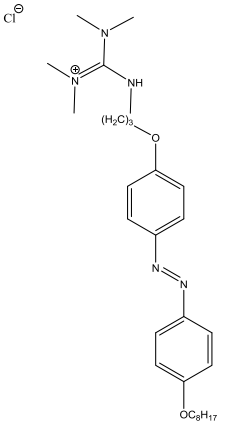

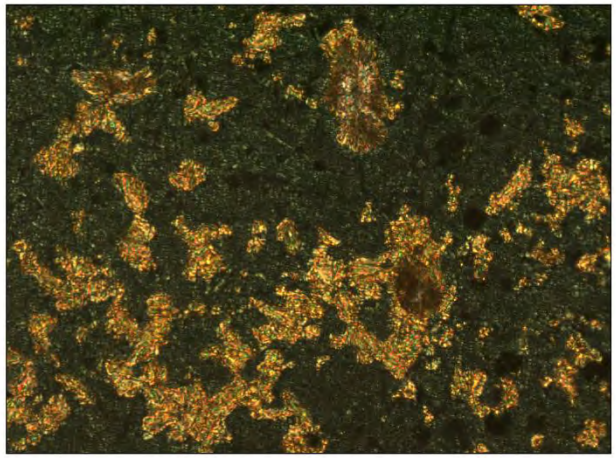

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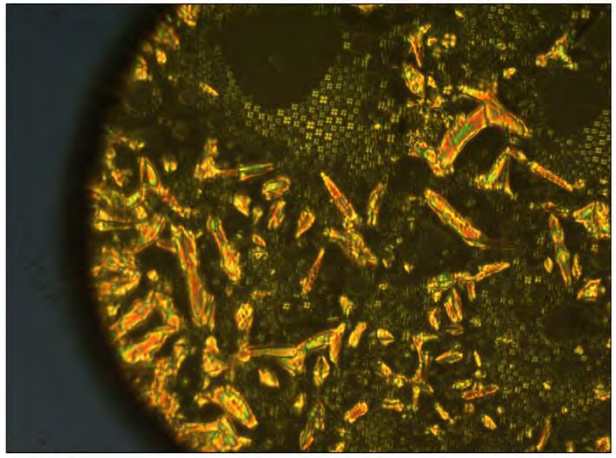

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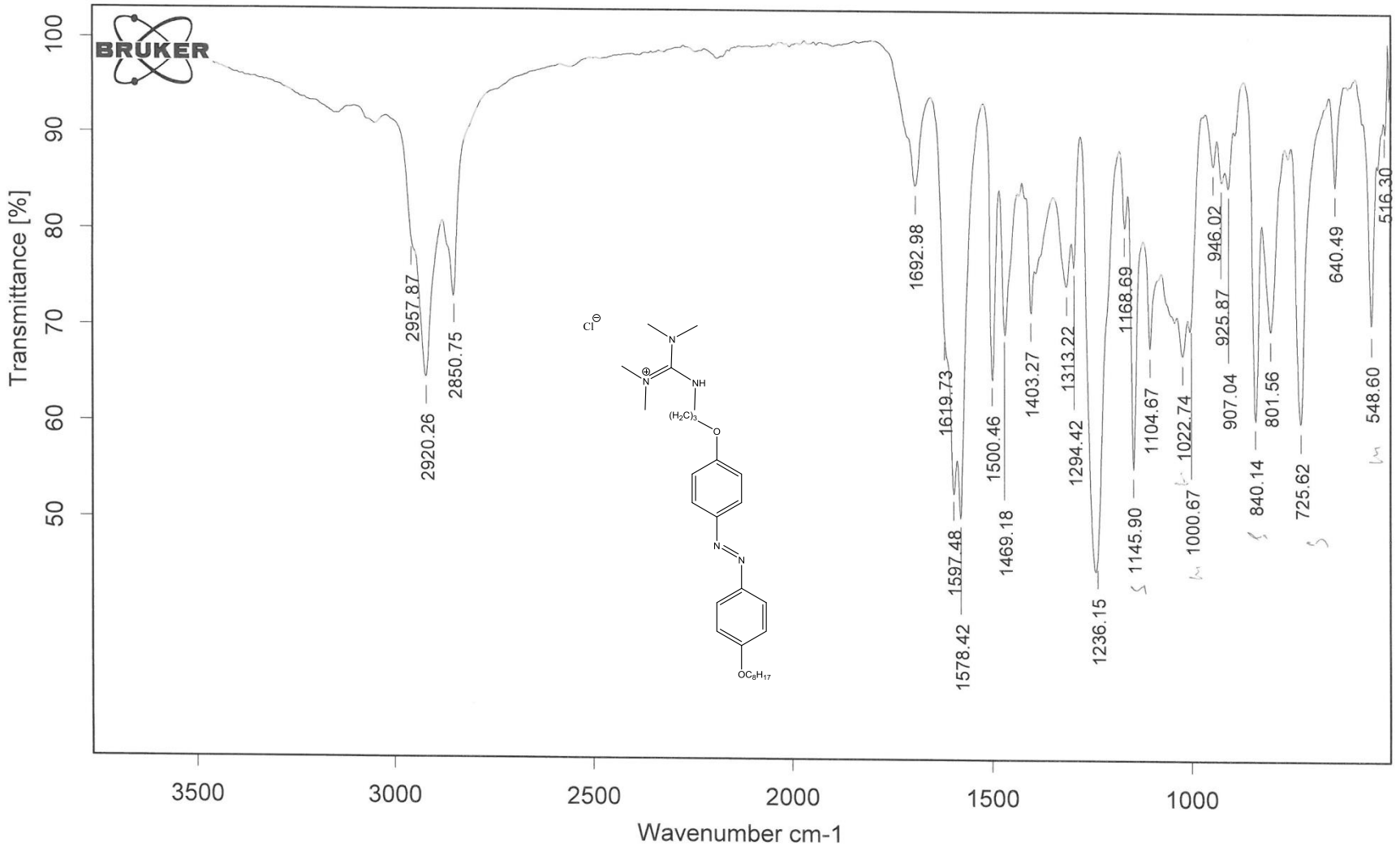
200x



D:\IR-DATEN\Wegner\940.0	Wuckert/940	fest	15/01/2014

Uncut

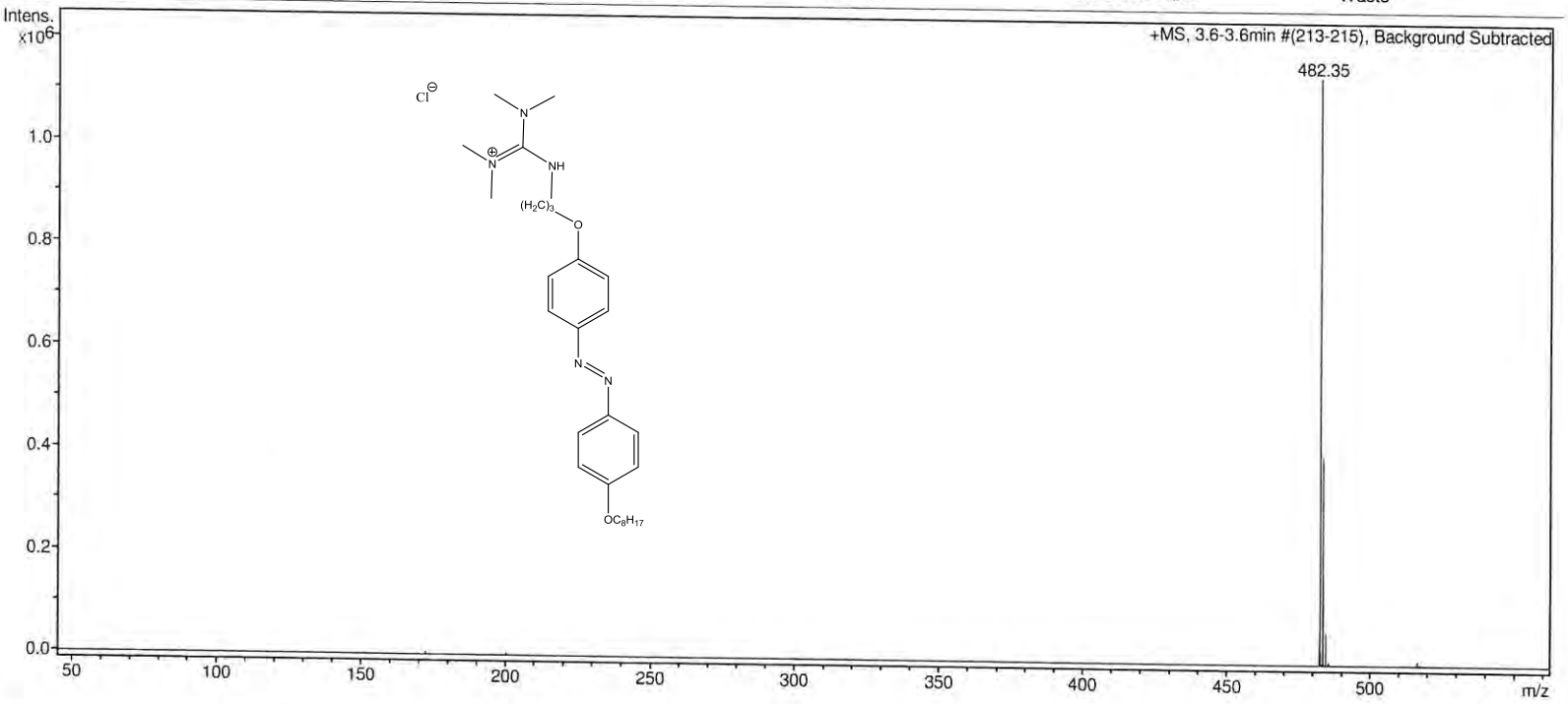
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	Laschat-Wuckert WUK940_4_01_19997.d	Acquisition Date	10.04.2013 09:15:44
Method	loop-tune-low.m		
Sample Name	Laschat-Wuckert WUK940	Operator	wo/tri
Comment		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



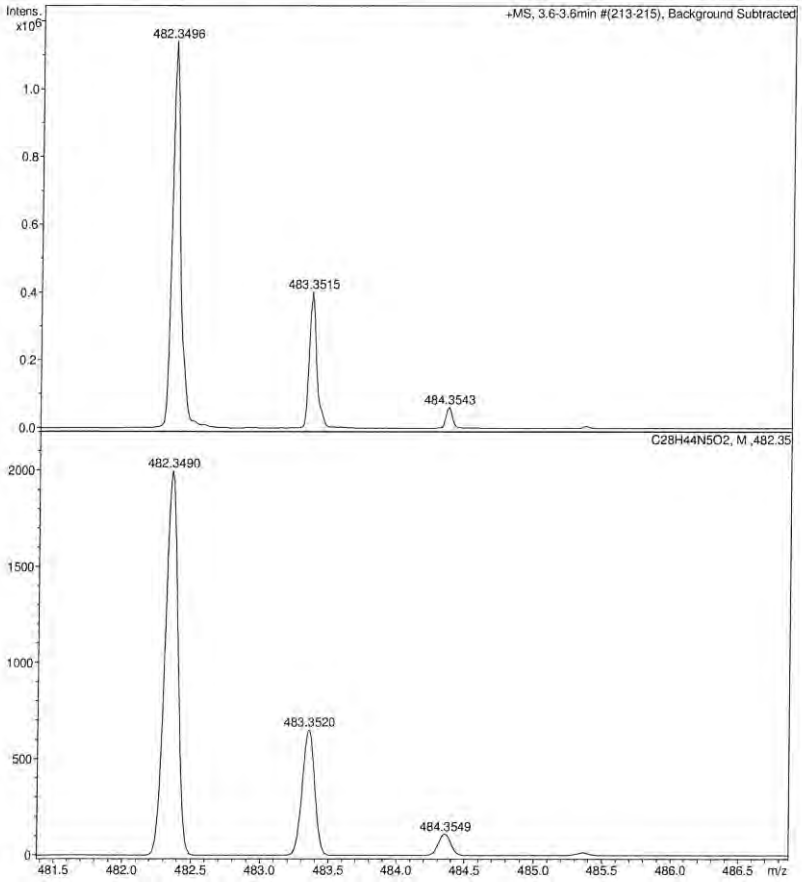
Massenspektrometrie - Universität Stuttgart

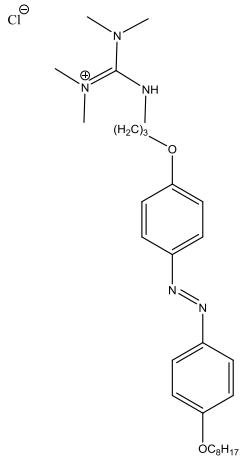
Analysis Info

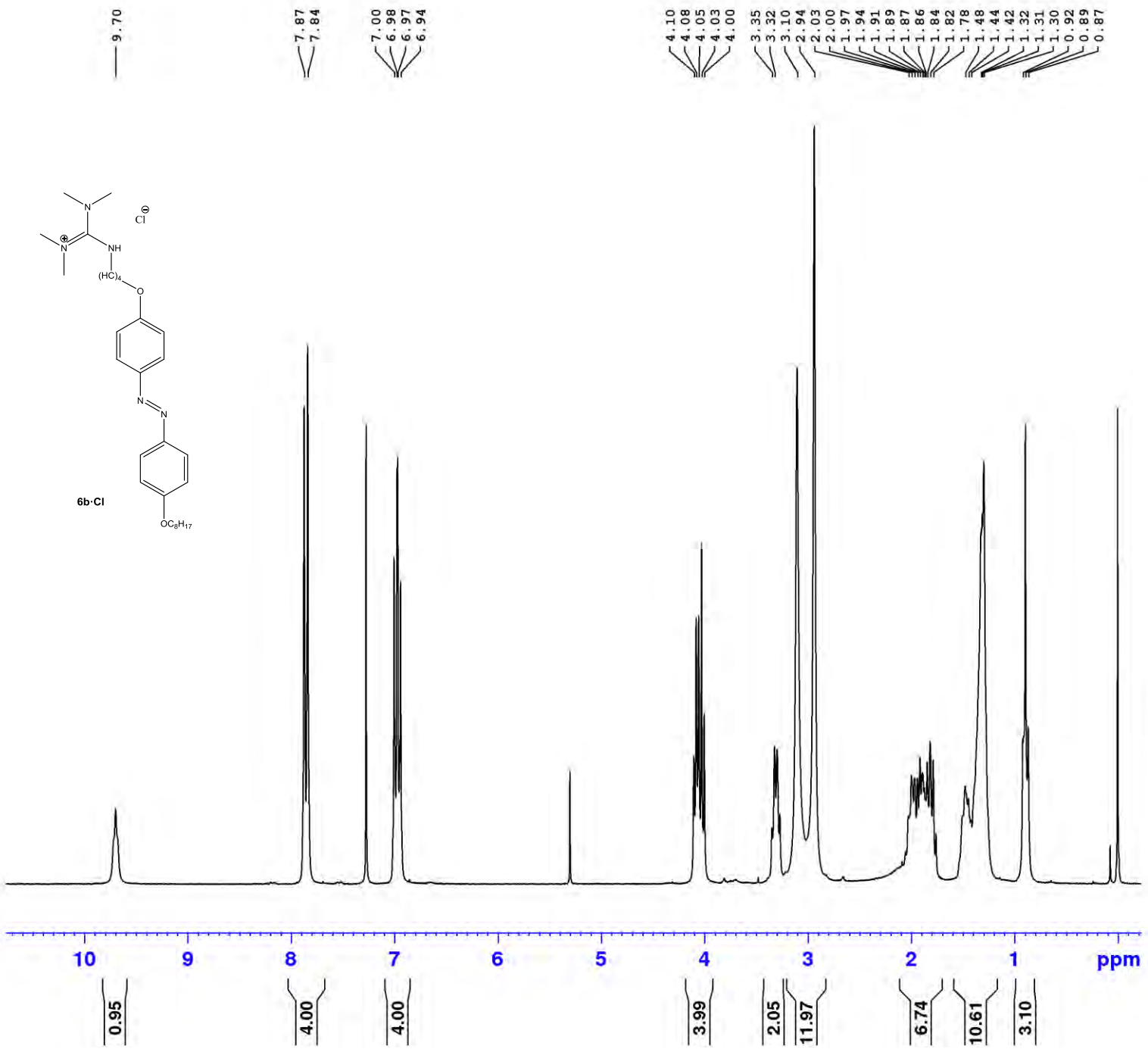
Analysis Name	Laschat-Wuckert WUK940_4_01_19997.d	Acquisition Date	10.04.2013 09:15:44
Method	loop-tune-low.m	Operator	wo/tri
Sample Name	Laschat-Wuckert WUK940	Instrument	micrOTOF-Q 43
Comment			

Acquisition Parameter

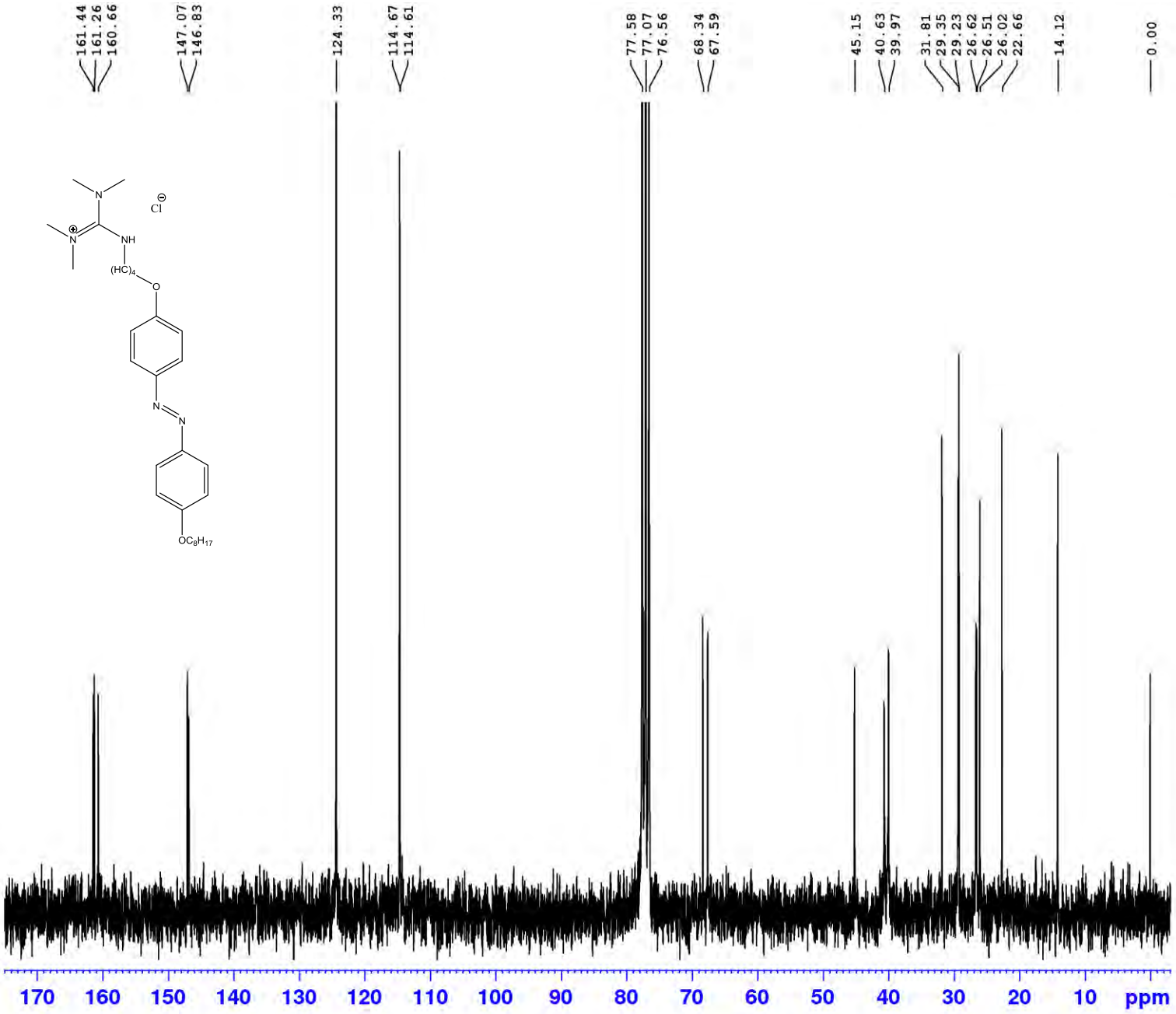
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste








```
Current Data Parameters
NAME                  Jun10-2013
EXPNO                        140
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20130610
Time                       13.49
INSTRUM                    spect
PROBHD     5 mm QNP 1H/13
PULPROG                     zg30
TD                         65536
SOLVENT                    CDCl3
NS                            32
DS                             2
SWH                     5175.983 Hz
FIDRES                  0.078979 Hz
AQ                      6.3307776 sec
RG                         322.5
DW                        96.600 usec
DE                         8.00 usec
TE                        300.0 K
D1                     1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                        10.40 usec
PL1                       -6.00 dB
SFO1                250.1315447 MHz

F2 - Processing parameters
SI                         65536
SF                  250.1300043 MHz
WDW                           EM
SSB                0
LB                        0.30 Hz
GB                 0
PC                        1.00
```




```
Current Data Parameters
NAME                  Jan13-2014
EXPNO                        151
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20140113
Time                       15.38
INSTRUM                    spect
PROBHD    5 mm QNP 1H/13
PULPROG                  zgpg30
TD                         65536
SOLVENT                    CDCl3
NS                          1024
DS                             4
SWH                  15060.241 Hz
FIDRES                0.229801 Hz
AQ                    2.1757953 sec
RG                          4096
DW                     33.200 usec
DE                      8.00 usec
TE                      300.0 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         13C
P1                     11.70 usec
PL1       0 dB
SFO1                 62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                         1H
PCPD2                  100.00 usec
PL2                     -6.00 dB
PL12                    18.50 dB
PL13                    15.00 dB
SFO2                250.1310005 MHz

F2 - Processing parameters
SI                           32768
SF                   62.8952401 MHz
WDW                             EM
SSB       0
LB                      1.00 Hz
GB        0
PC                      1.40
```

^exo wuk 1112.2_3x integriert 18.09.2014 15:36:20

Methodenname: wuk 25...160...25_3x

[]8[wuk 1112.2
wuk 1112.2, 2,9900 mg 3.Kühlen

Kühlen

Integral 139,88 mJ
normalis. 46,78 Jg^-1

Integral 5,60 mJ
normalis. 1,87 Jg^-1

Onset 109,14 °C

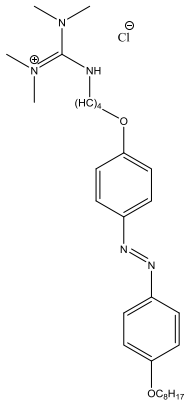
Onset 153,05 °C

10
mW

Heizen

[]7[wuk 1112.2
wuk 1112.2, 2,9900 mg

3.Heizen



Onset 125,40 °C

Onset 151,06 °C

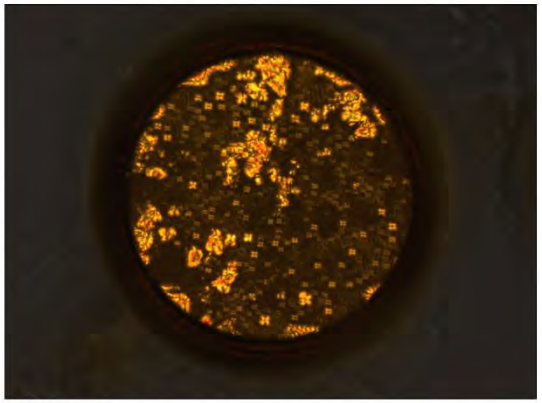
Integral -156,90 mJ
normalis. -52,48 Jg^-1

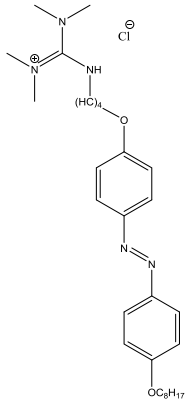
Integral -5,78
normalis. -1,93

30 40 50 60 70 80 90 100 110 120 130 140 150 °C

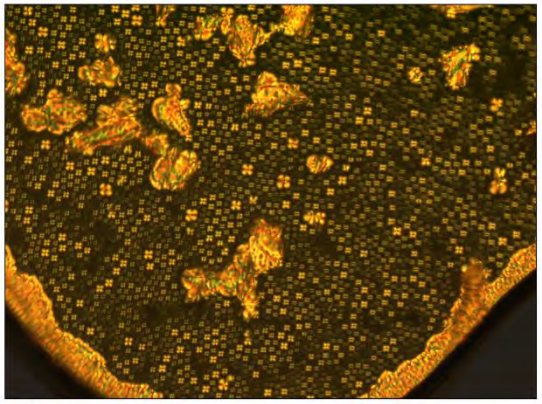
Uni Stuttgart - AK Laschat: Wuckert METTLER TOLEDO STARe SW 7.01

8 Sp4 (wuk 834, 855)

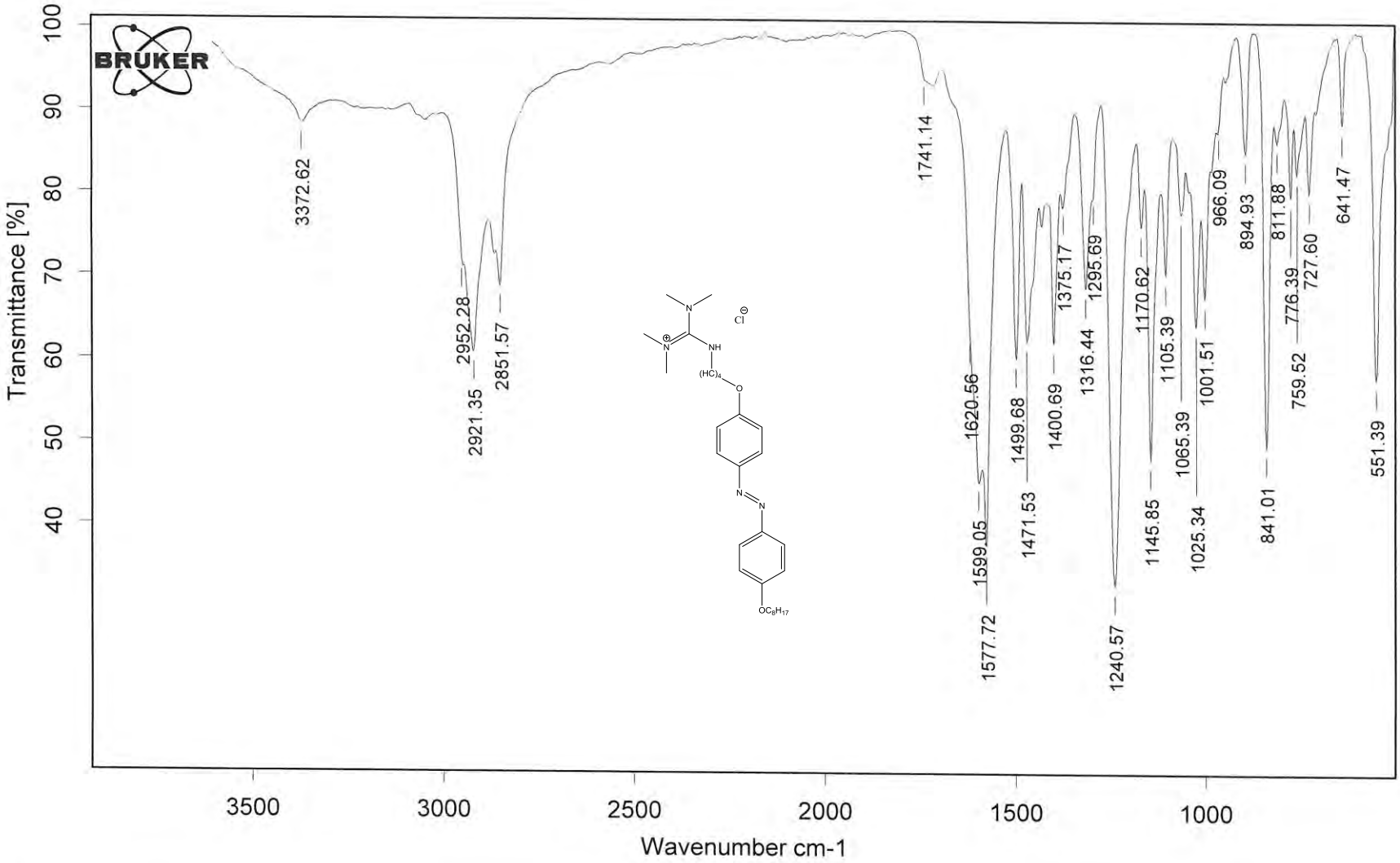




Bildname: wuk 855 (50 mg Ch).1
Bildkommentar: isotrop bei 161°, bei gleicher Temp. nach einigen Min. entstehen Texturen
200x



Bildname: wuk 834 (wahrsch. NMR-Ch)
Bildkommentar: Heizen - bei 158° - isotrop
Kühlen 1°/min bei 157°
200x



D:\IR-DATEN\Wegner\950.H2O.0	Wuckert/950.H2O	fest	15/01/2014

Wuckert

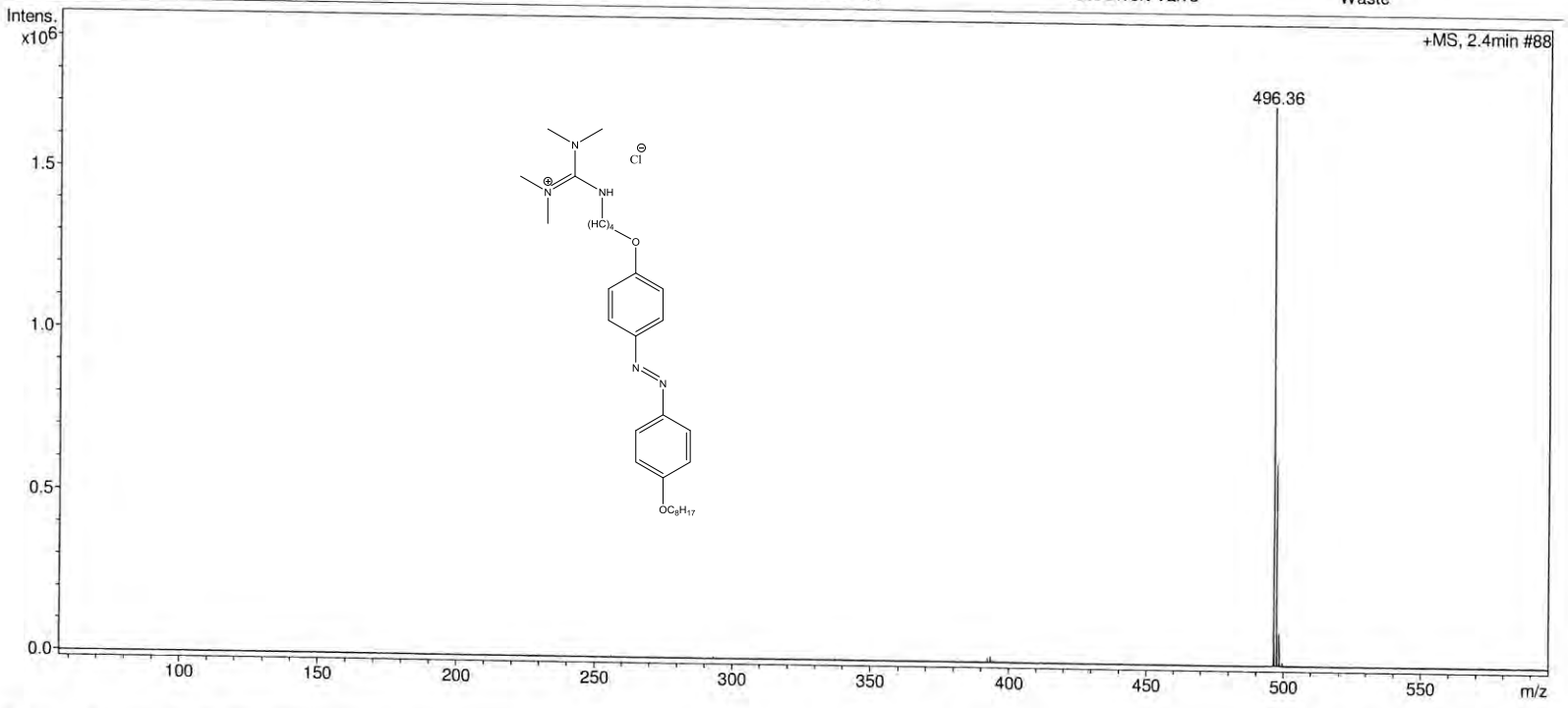
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	Laschat-Wuckert WUK 834 + 855_3_01_18445.d	Acquisition Date	19.10.2012 09:09:20
Method	loop-tune-low.m		
Sample Name	Laschat-Wuckert WUK 834 + 855	Operator	wo/tri
Comment		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



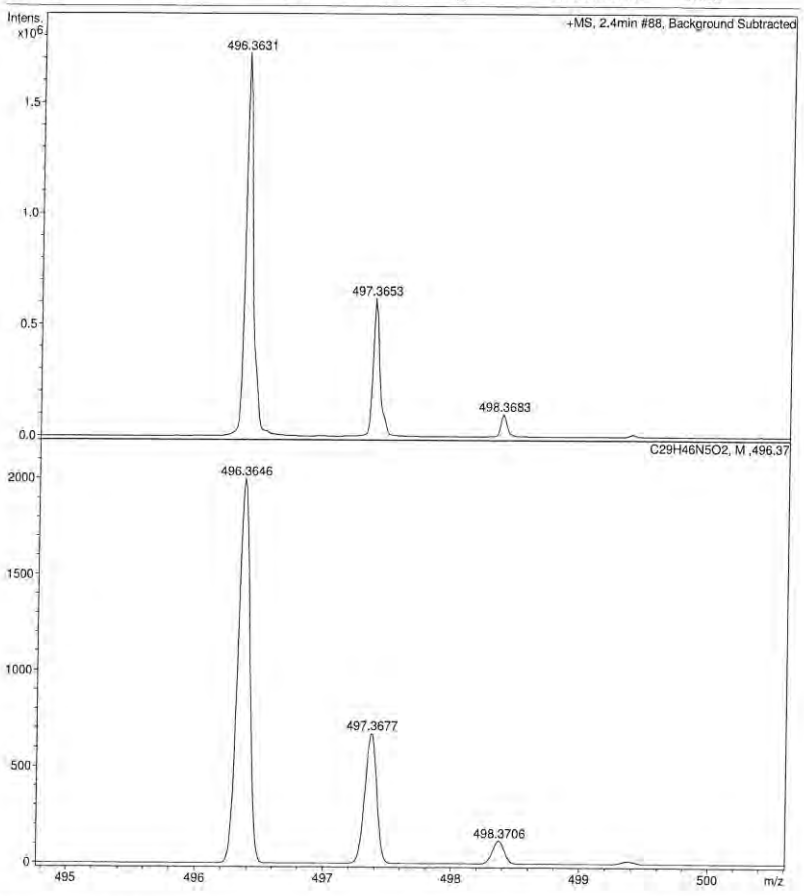
Massenspektrometrie - Universität Stuttgart

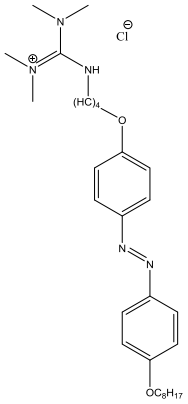
Analysis Info

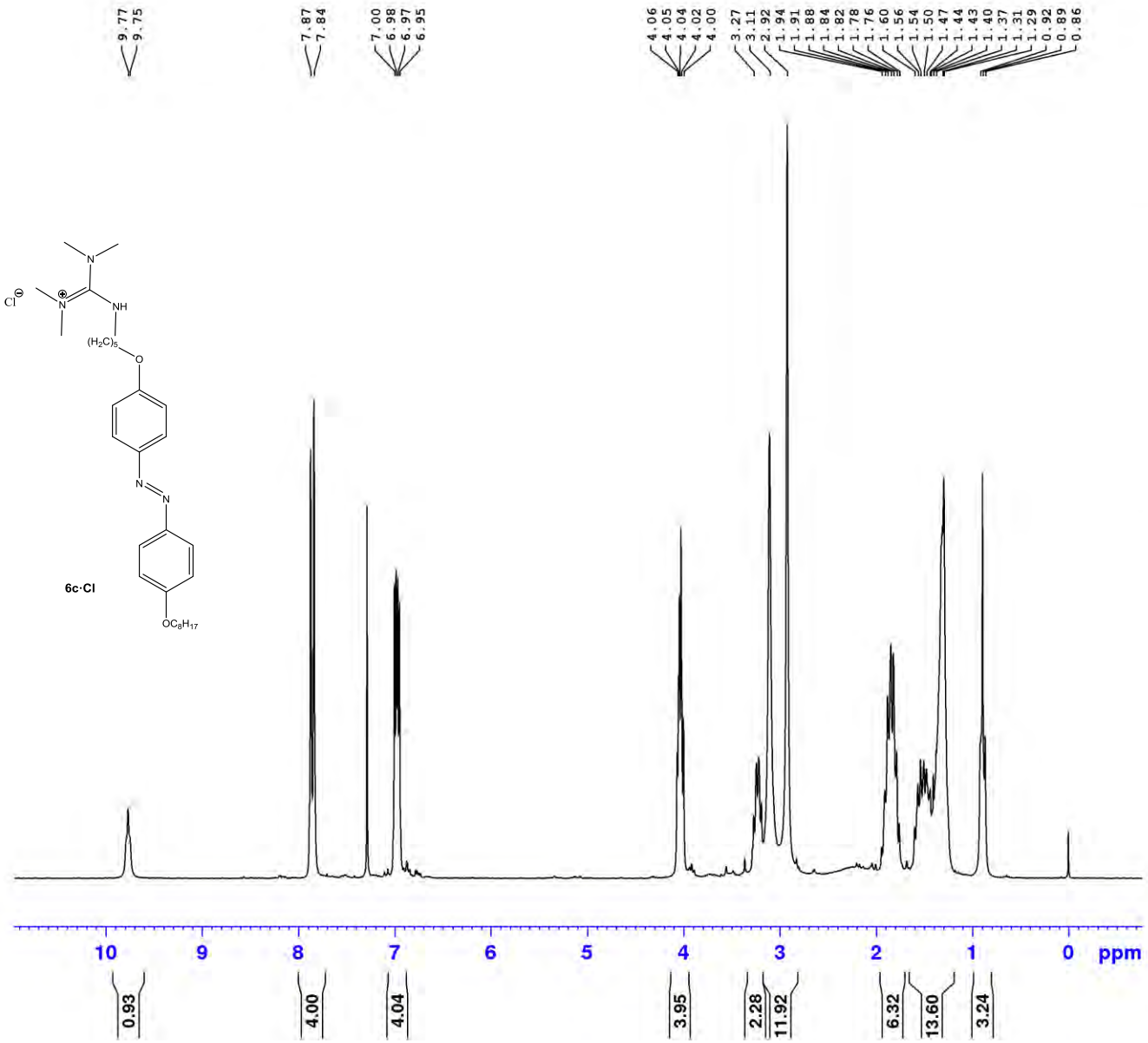
Analysis Name	Laschat-Wuckert WUK 834 + 855_3_01_18445.d	Acquisition Date	19.10.2012 09:09:20
Method	loop-tune-low.m	Operator	wo/tri
Sample Name	Laschat-Wuckert WUK 834 + 855	Instrument	micrOTOF-Q 43
Comment			

Acquisition Parameter

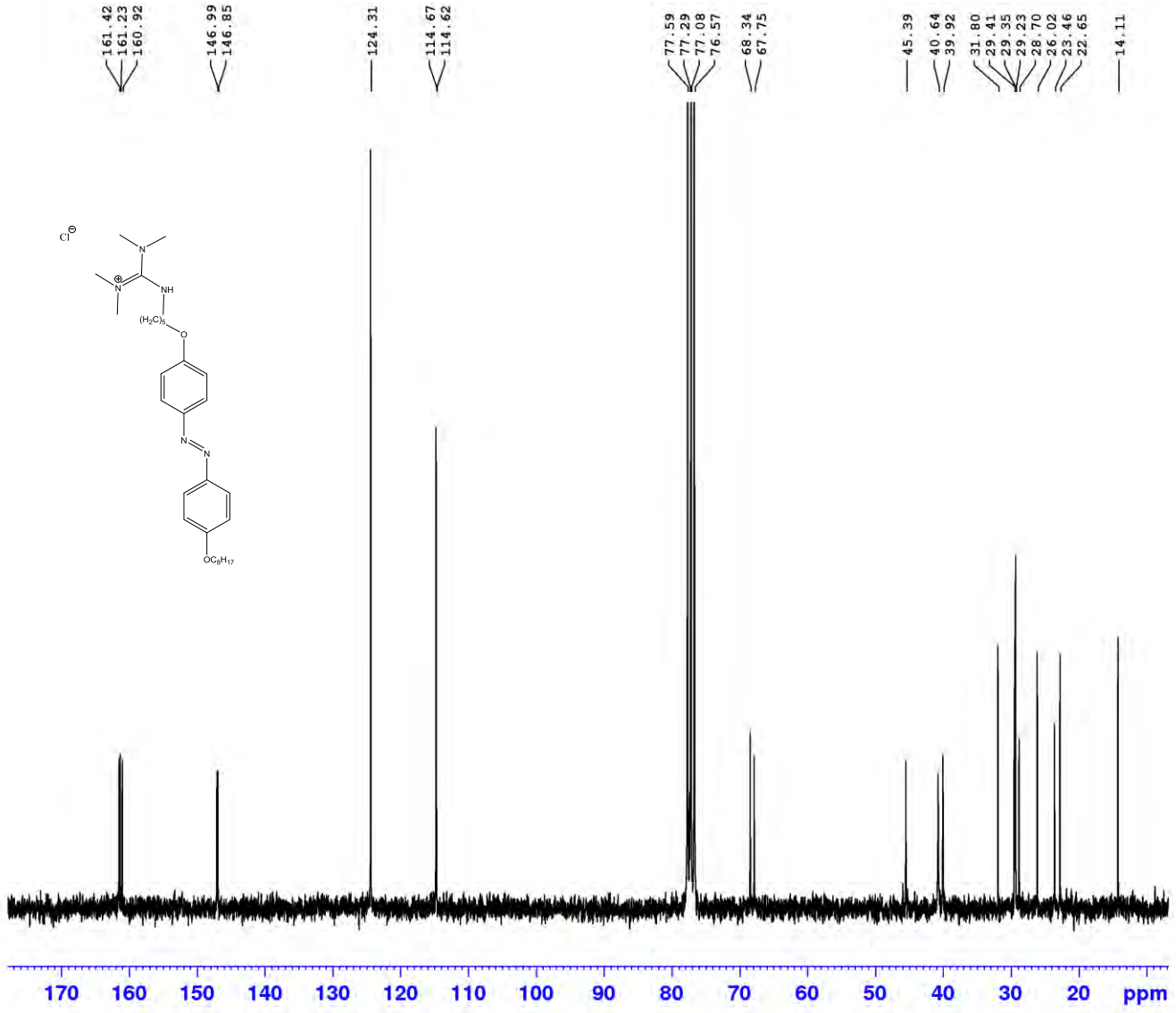
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste





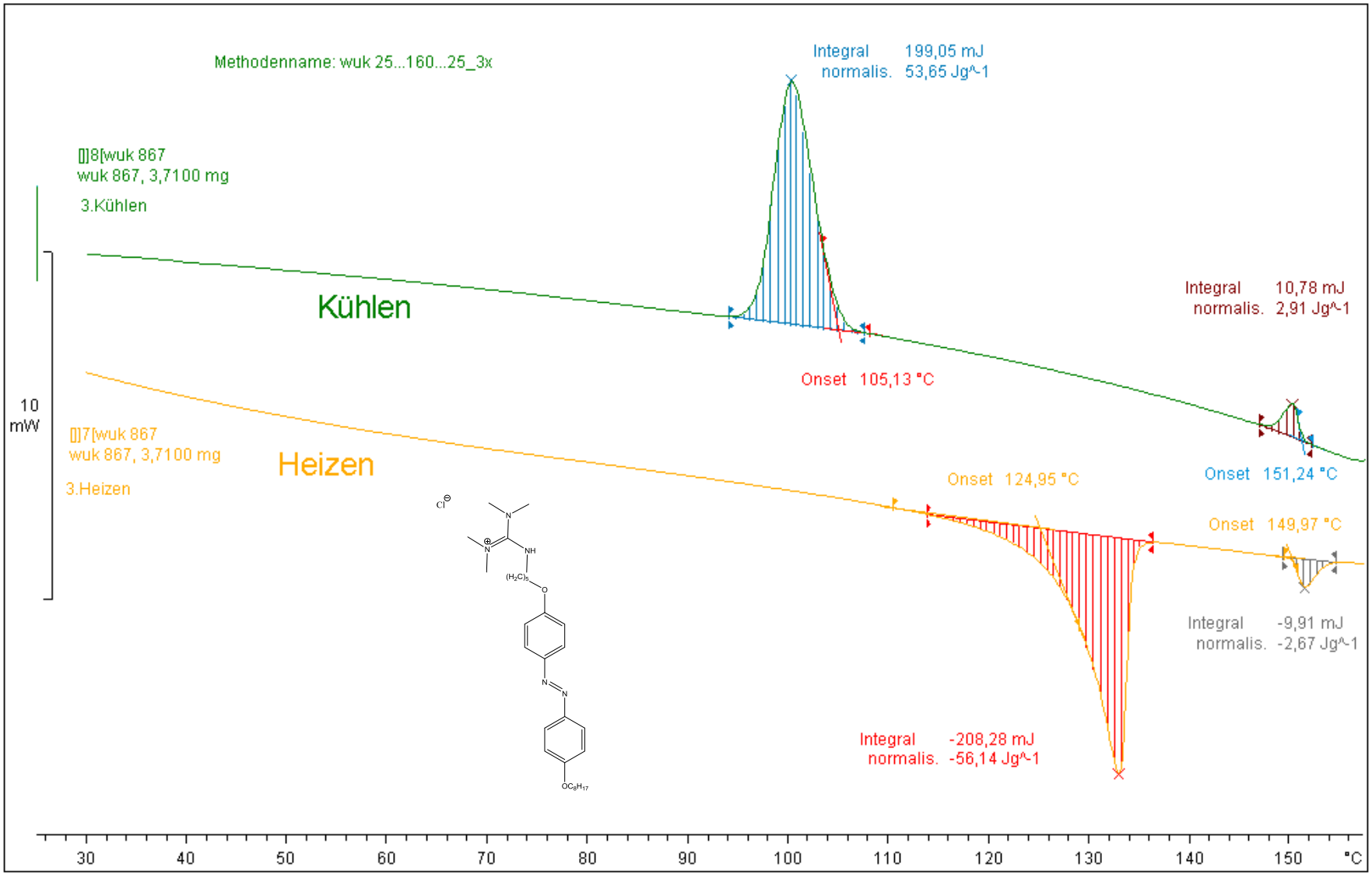



```
Current Data Parameters
NAME          Sep24-2012
EXPNO                 70
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120924
Time               15.44
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     2
SWH            5175.983 Hz
FIDRES        0.078979 Hz
AQ            6.3307776 sec
RG                228.1
DW               96.600 usec
DE                8.00 usec
TE                300.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.40 usec
PL1               -6.00 dB
SFO1         250.1315447 MHz

F2 - Processing parameters
SI                 65536
SF           250.1300013 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



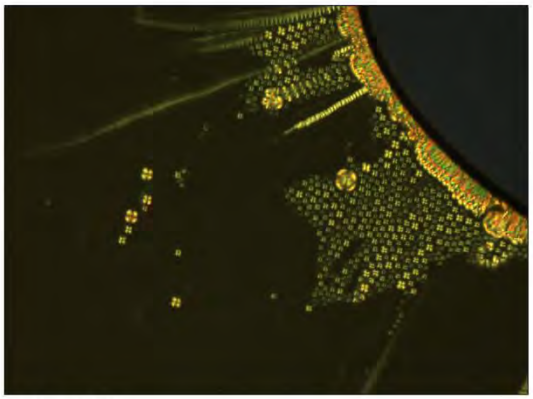

```
Current Data Parameters
NAME          Sep24-2012
EXPNO                 71
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120924
Time               16.58
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDC13
NS                 1024
DS                    4
SWH           15060.241 Hz
FIDRES         0.229801 Hz
AQ            2.1757953 sec
RG               2896.3
DW                33.200 usec
DE                 8.00 usec
TE                300.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 11.70 usec
PL1       0 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2             100.00 usec
PL2                -6.00 dB
PL12               18.50 dB
PL13               15.00 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                 32768
SF           62.8952350 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

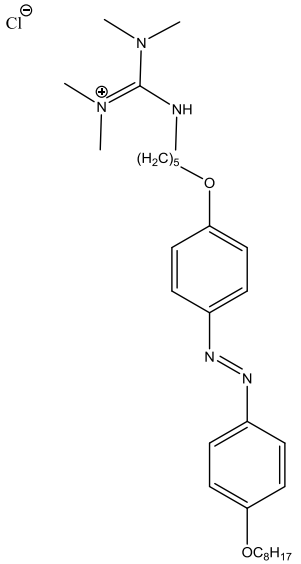
^exo wuk 867 3x integriert 18.09.2014 15:37:41



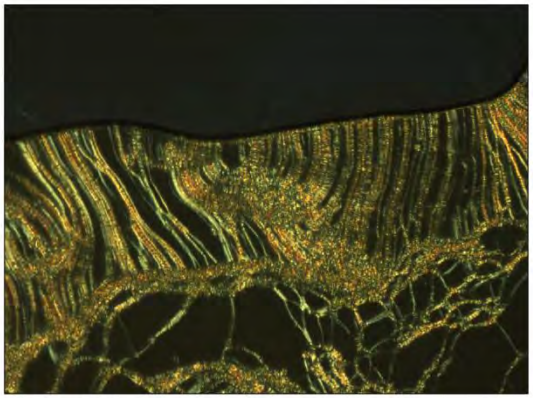
Uni Stuttgart - AK Laschat: Wuckert METTLER TOLEDO STAR^{e} SW 7.01

8 Sp 5 (wuk 867)

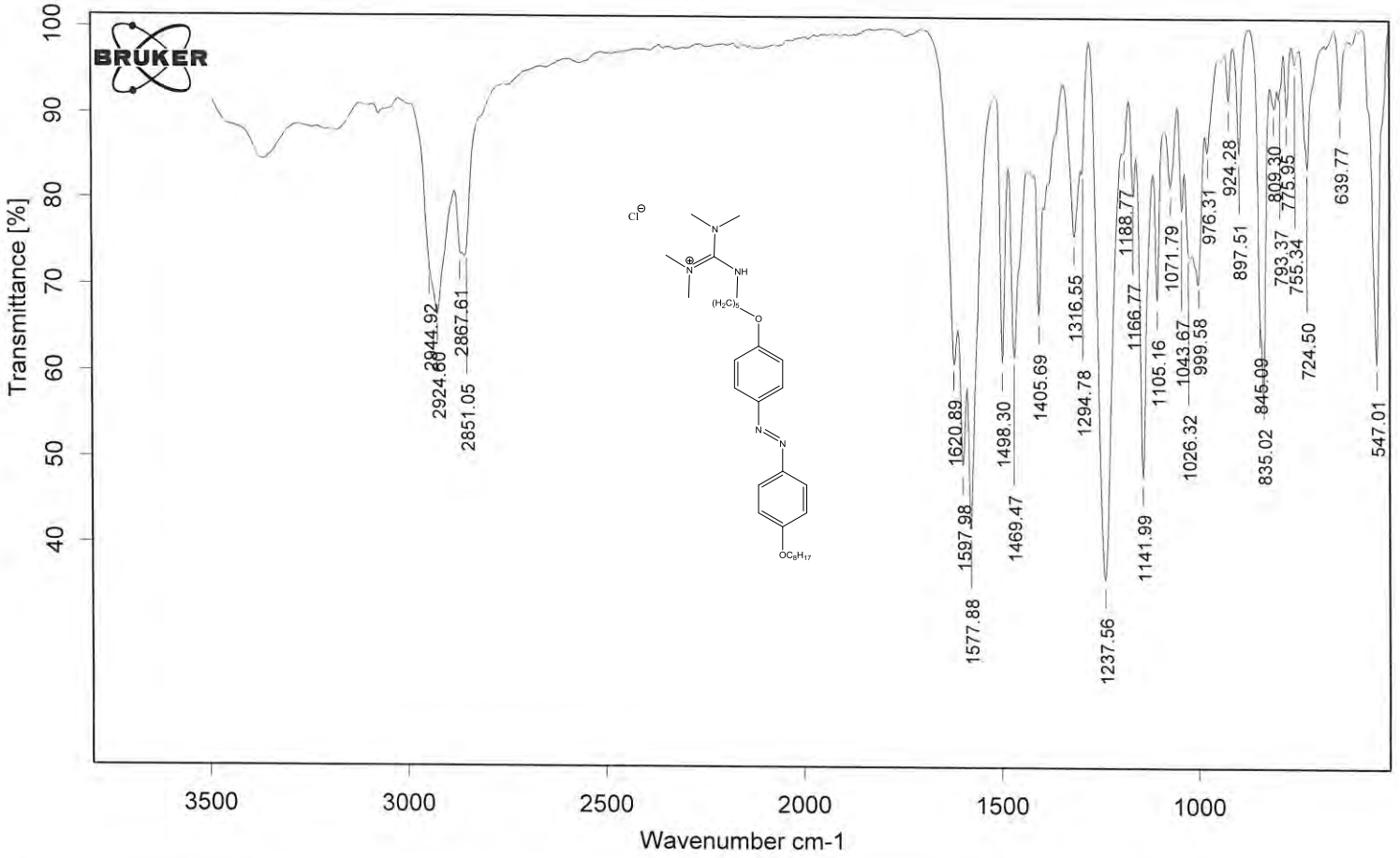




Bildname: wuk 867.5.3 Cr MeCN
Bildkommentar: Kühlen, von ca. 150° mit 10°/min dann mit 5, 1°/min
bei 128°
200x



Bildname: wuk 867.5.4 Cr MeCN
Bildkommentar: Kühlen, von ca. 150° mit 10°/min dann mit 5°, 3°/min
bei 105°
200x



D:\IR-DATEN\Wegner\8sp7 867.0	Wuckert/8sp7 867	fest	15/01/2014

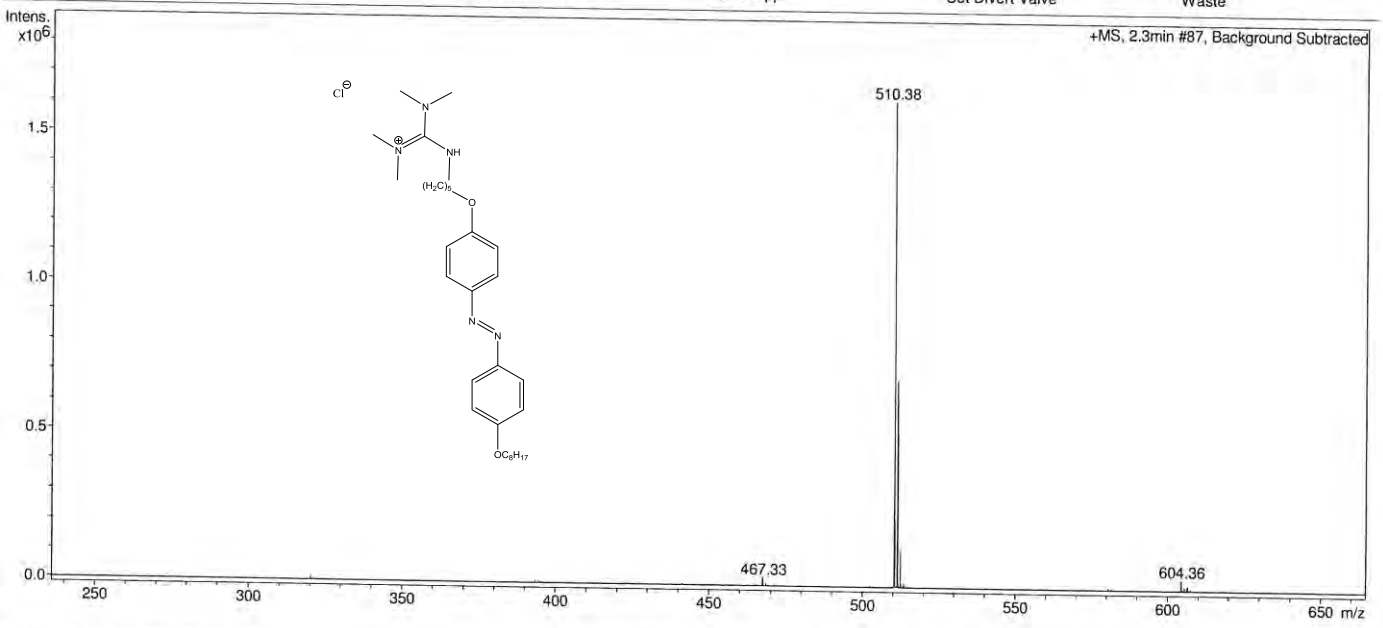
Massenspektrometrie - Universität Stuttgart

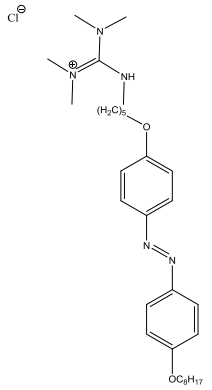
Analysis Info

Analysis Name	Laschat-Wuckert WUK 867 MLMeCN_9_01_18457.d	Acquisition Date	19.10.2012 10:23:44
Method	test-withloop.m		
Sample Name	Laschat-Wuckert WUK 867 MLMeCN	Operator	wo/tri
Comment		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	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	580.0 Vpp	Set Divert Valve	Waste





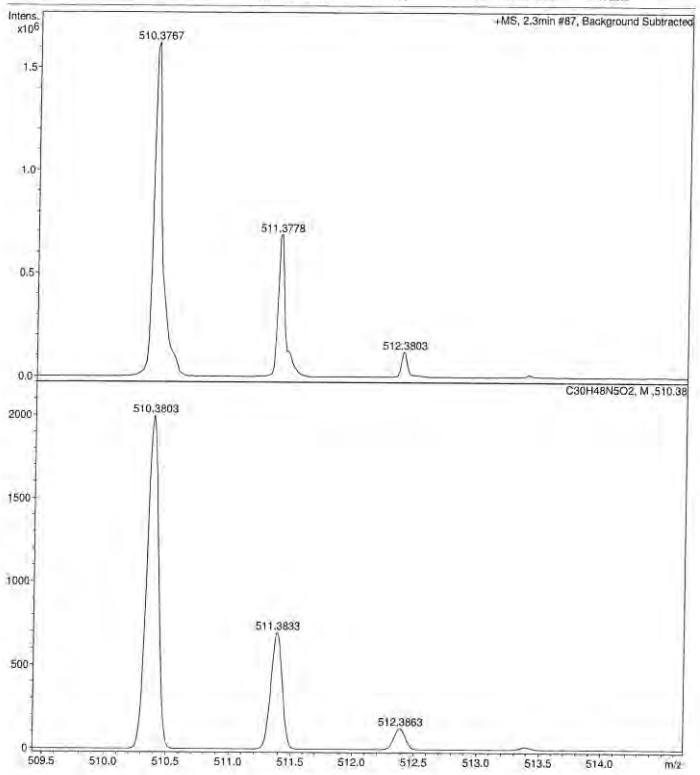
Massenspektrometrie - Universität Stuttgart

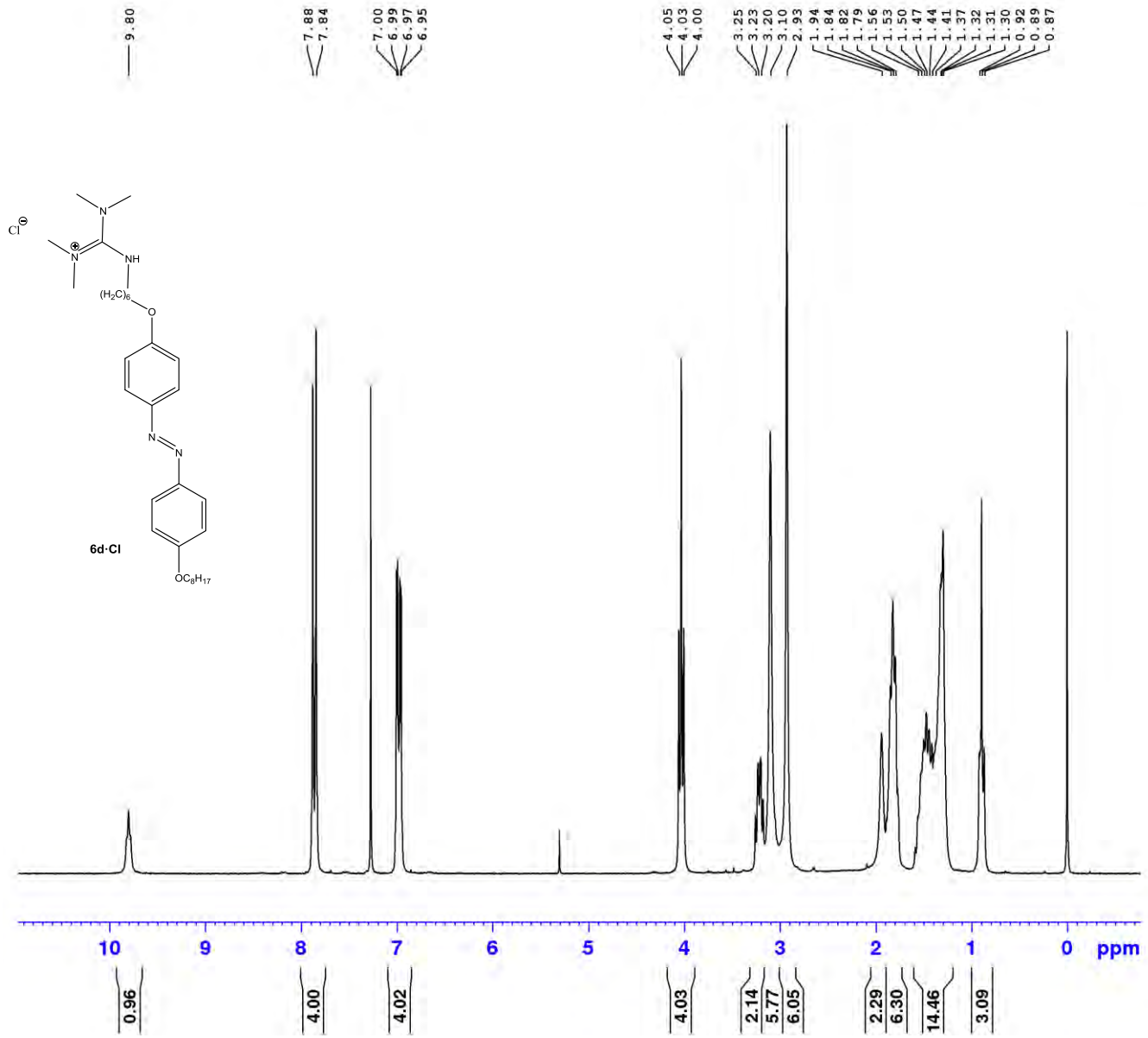
Analysis Info

Analysis Name	Laschat-Wuckert WUK 867 MLMeCN_9_01_18457.d	Acquisition Date	19.10.2012 10:23:44
Method	test-withloop.m	Operator	wo/tri
Sample Name	Laschat-Wuckert WUK 867 MLMeCN	Instrument	micrOTOF-Q 43
Comment			

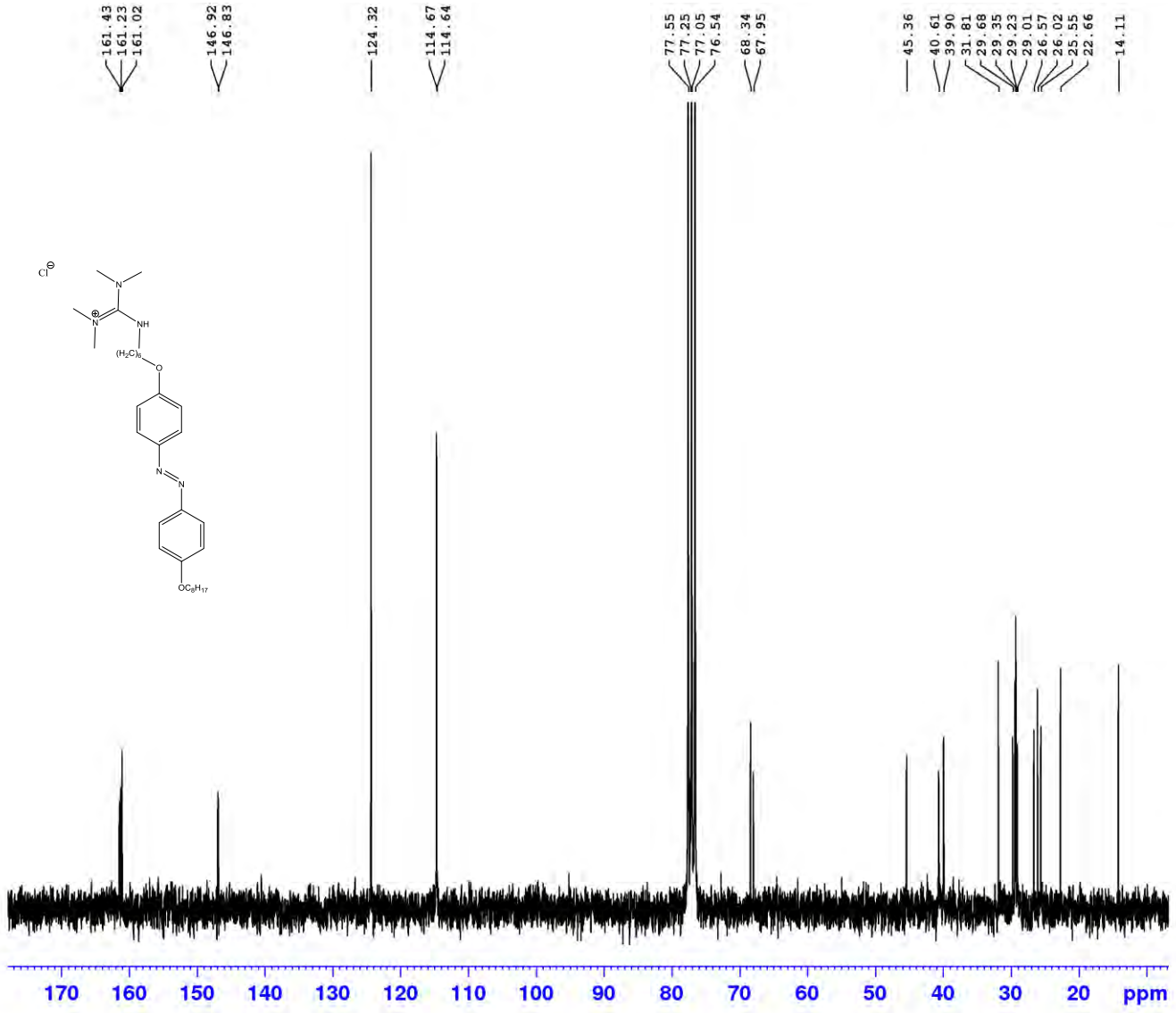
Acquisition Parameter

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	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	580.0 Vpp	Set Divert Valve	Waste

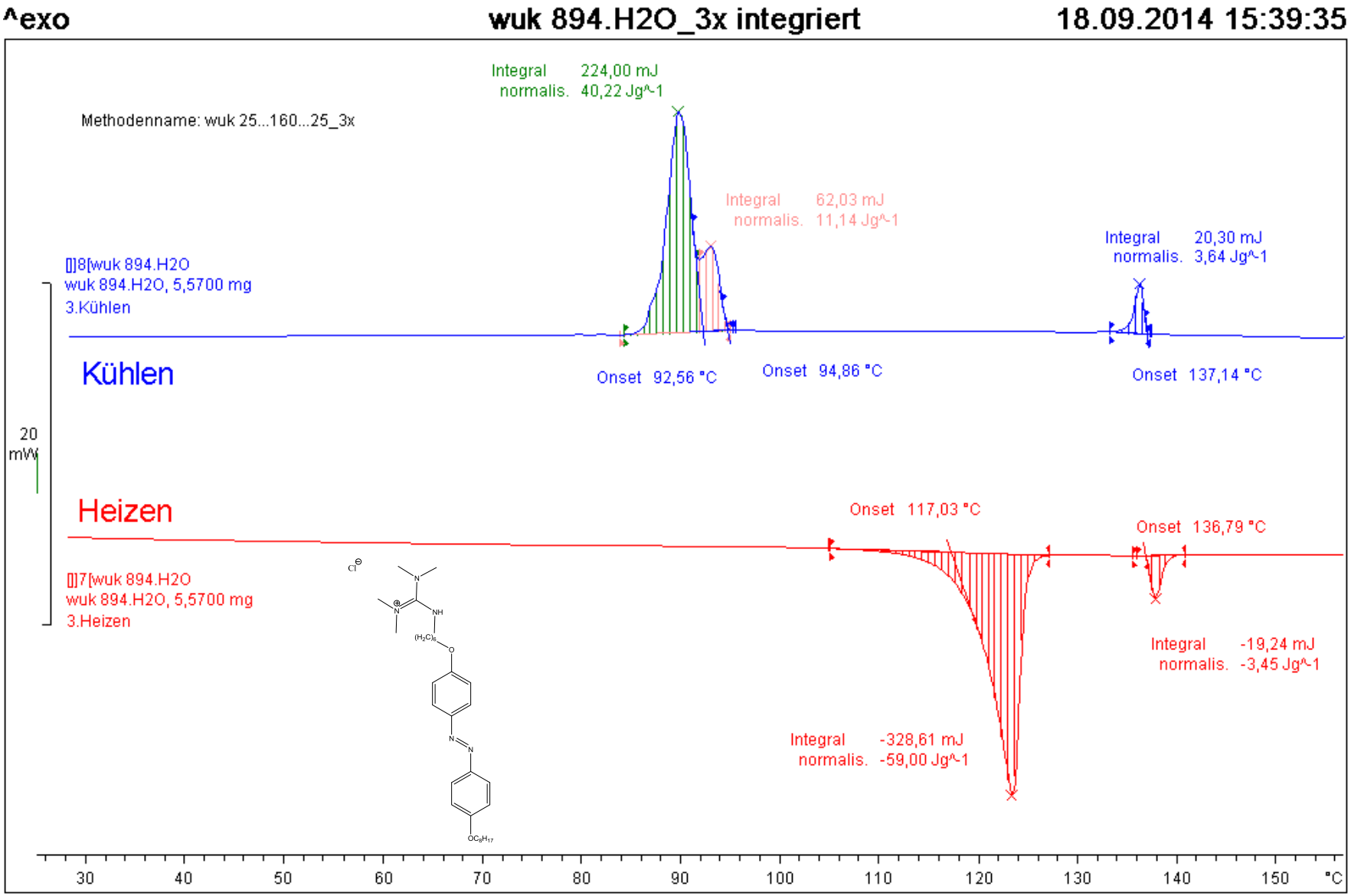


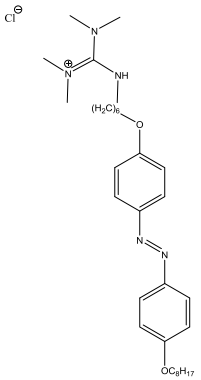


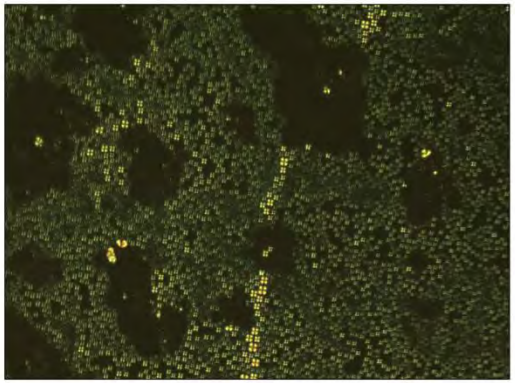

```
Current Data Parameters
NAME                  Jun13-2013
EXPNO                        100
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20130613
Time                       10.57
INSTRUM                    spect
PROBHD    5 mm QNP 1H/13
PULPROG                     zg30
TD                         65536
SOLVENT                    CDCl3
NS                            32
DS                             2
SWH                     5175.983 Hz
FIDRES                  0.078979 Hz
AQ                    6.3307776 sec
RG                           362
DW                        96.600 usec
DE                         8.00 usec
TE                        300.0 K
D1                    1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                        10.40 usec
PL1                       -6.00 dB
SFO1                250.1315447 MHz

F2 - Processing parameters
SI                         65536
SF                  250.1300047 MHz
WDW                           EM
SSB                0
LB                         0.30 Hz
GB                 0
PC                         1.00
```



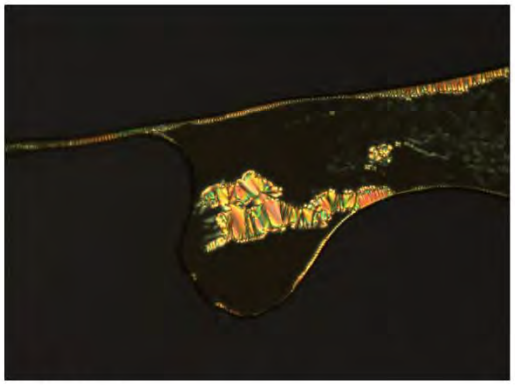

```
Current Data Parameters
NAME                  Jun13-2013
EXPNO                        101
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20130613
Time                       19.13
INSTRUM                    spect
PROBHD   5 mm QNP 1H/13
PULPROG                  zgpg30
TD                          65536
SOLVENT                     CDC13
NS                           1024
DS                              4
SWH                  15060.241 Hz
FIDRES                0.229801 Hz
AQ                    2.1757953 sec
RG                       2896.3
DW                        33.200 usec
DE                         8.00 usec
TE                        300.0 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                         13C
P1                         11.70 usec
PL1       0 dB
SFO1                62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                         1H
PCPD2                    100.00 usec
PL2                       -6.00 dB
PL12                      18.50 dB
PL13                      15.00 dB
SFO2                250.1310005 MHz

F2 - Processing parameters
SI                           32768
SF                  62.8952395 MHz
WDW                             EM
SSB       0
LB                         1.00 Hz
GB        0
PC                         1.40
```


^exo
wuk 894.H2O_3x integriert
18.09.2014 15:39:35
Integral 224,00 mJ
normalis. 40,22 Jg^-1
Methodenname: wuk 25...160...25_3x
Integral 62,03 mJ
normalis. 11,14 Jg^-1
Integral 20,30 mJ
normalis. 3,64 Jg^-1
[]8[wuk 894.H2O
wuk 894.H2O, 5,5700 mg
3.Kühlen
Kühlen
Onset 92,56 °C
Onset 94,86 °C
Onset 137,14 °C
20
mW
Heizen
Onset 117,03 °C
Onset 136,79 °C
[]7[wuk 894.H2O
wuk 894.H2O, 5,5700 mg
3.Heizen
Integral -19,24 mJ
normalis. -3,45 Jg^-1
Integral -328,61 mJ
normalis. -59,00 Jg^-1
30
40
50
60
70
80
90
100
110
120
130
140
150
°C
Uni Stuttgart - AK Laschat: Wuckert
METTLER TOLEDO STARe SW 7.01

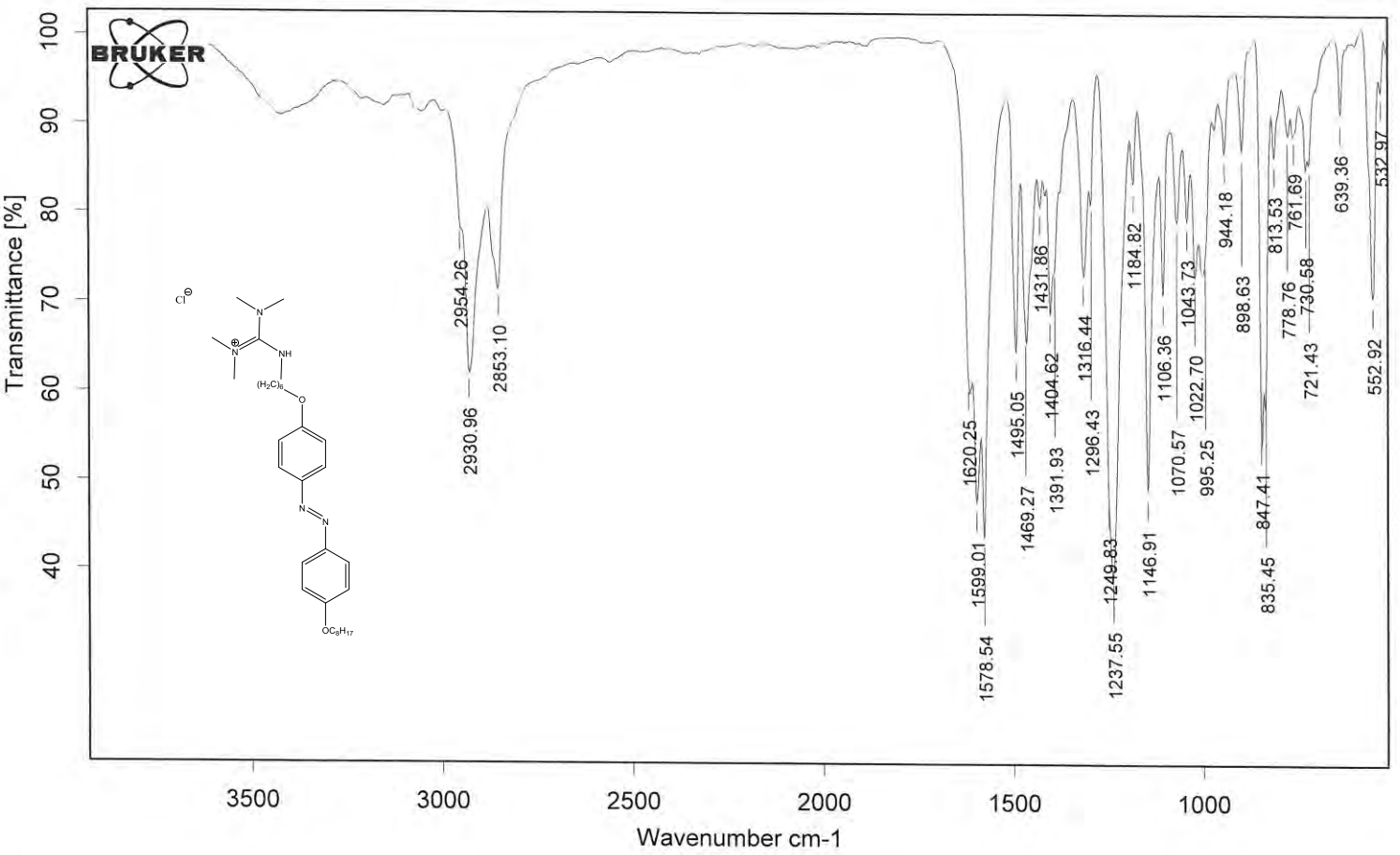




Bildname: wuk 877.3
Bildkommentar: Kühlen d. Schmelze (ca. 155°) mit 5°/min
bei 135,7°
200x



Bildname: wuk 877.3 (THF-Extr.)
Bildkommentar: Kühlen der isotropen Phase (145°) mit 1°/min
bei 130°
200x



D:\IR-DATEN\Wegner\894.H2O.1+2 85p6.0	Wuckert/894.H2O.1+2 85p6	fest	15/01/2014

Wuckert

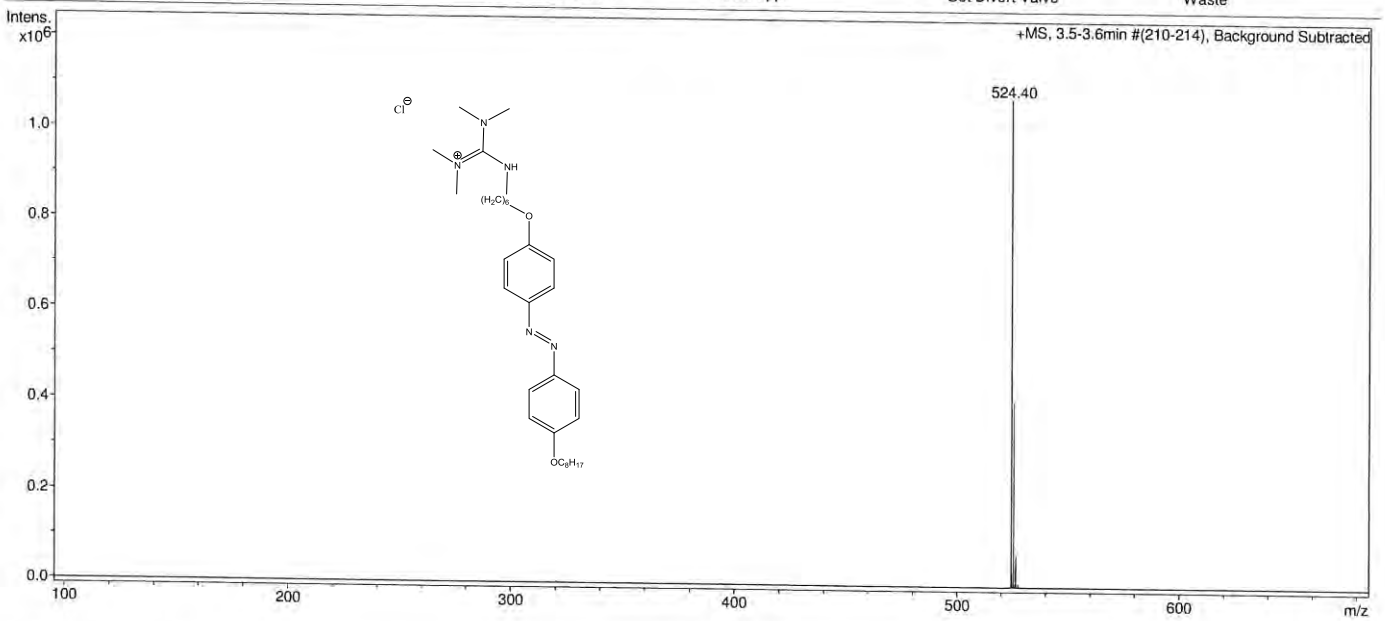
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	Laschat-Wuckert WUK 877_3_01_18758.d	Acquisition Date	22.11.2012 14:03:57
Method	loop-tune-low.m		
Sample Name	Laschat-Wuckert WUK 877	Operator	wo/tri
Comment		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



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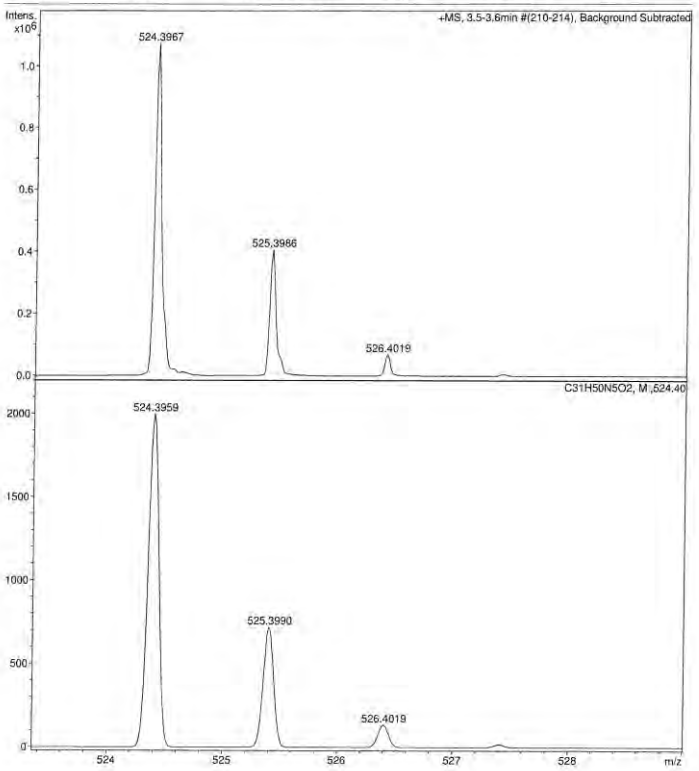
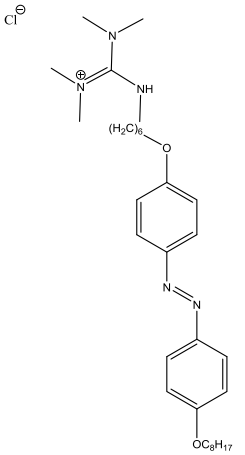
Analysis Info

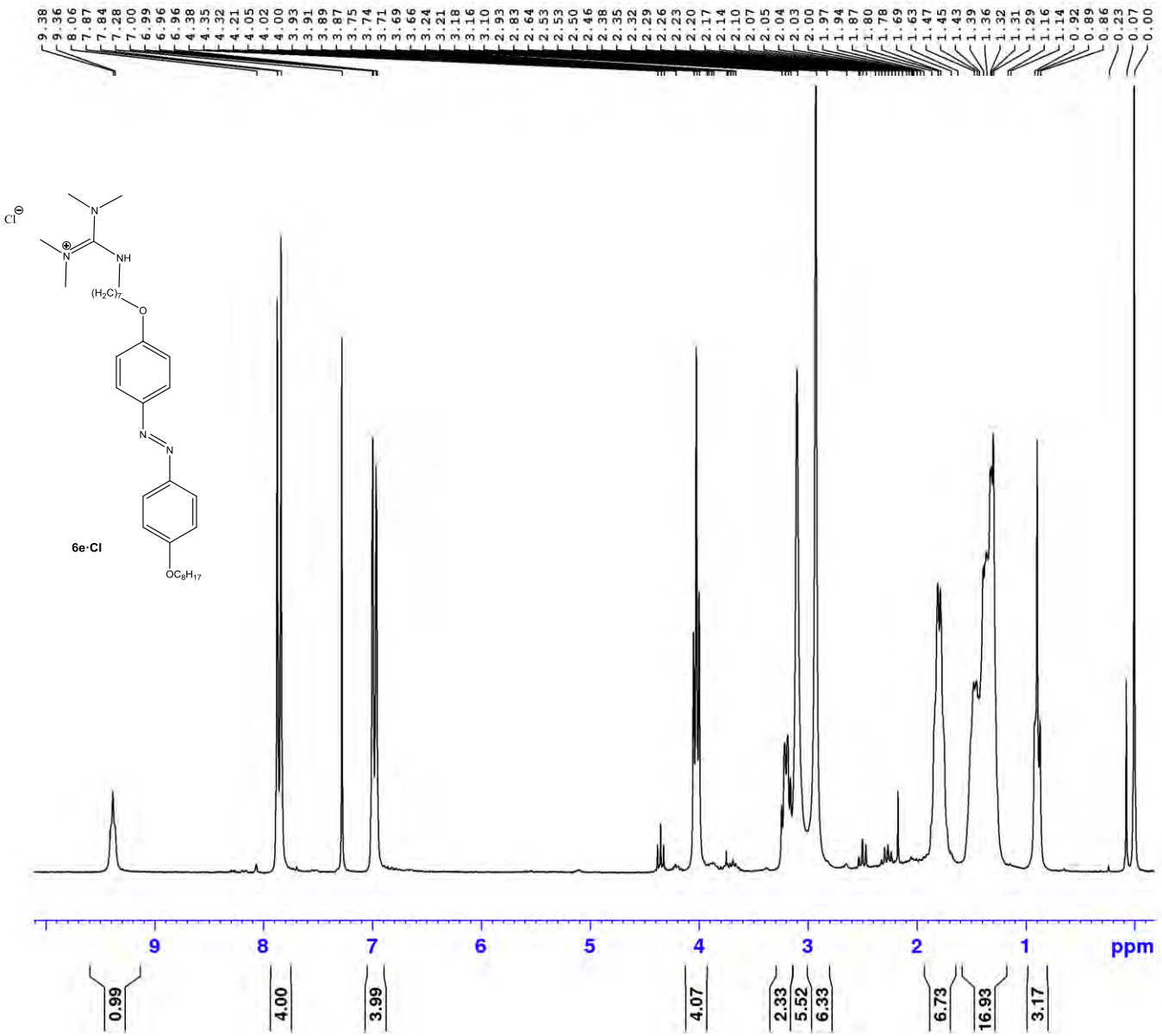
Analysis Name	Laschat-Wuckert WUK 877_3_01_18758.d	Acquisition Date	22.11.2012 14:03:57
Method	loop-tune-low.m	Operator	wo/tri
Sample Name	Laschat-Wuckert WUK 877	Instrument	micrOTOF-Q 43
Comment			

Acquisition Parameter

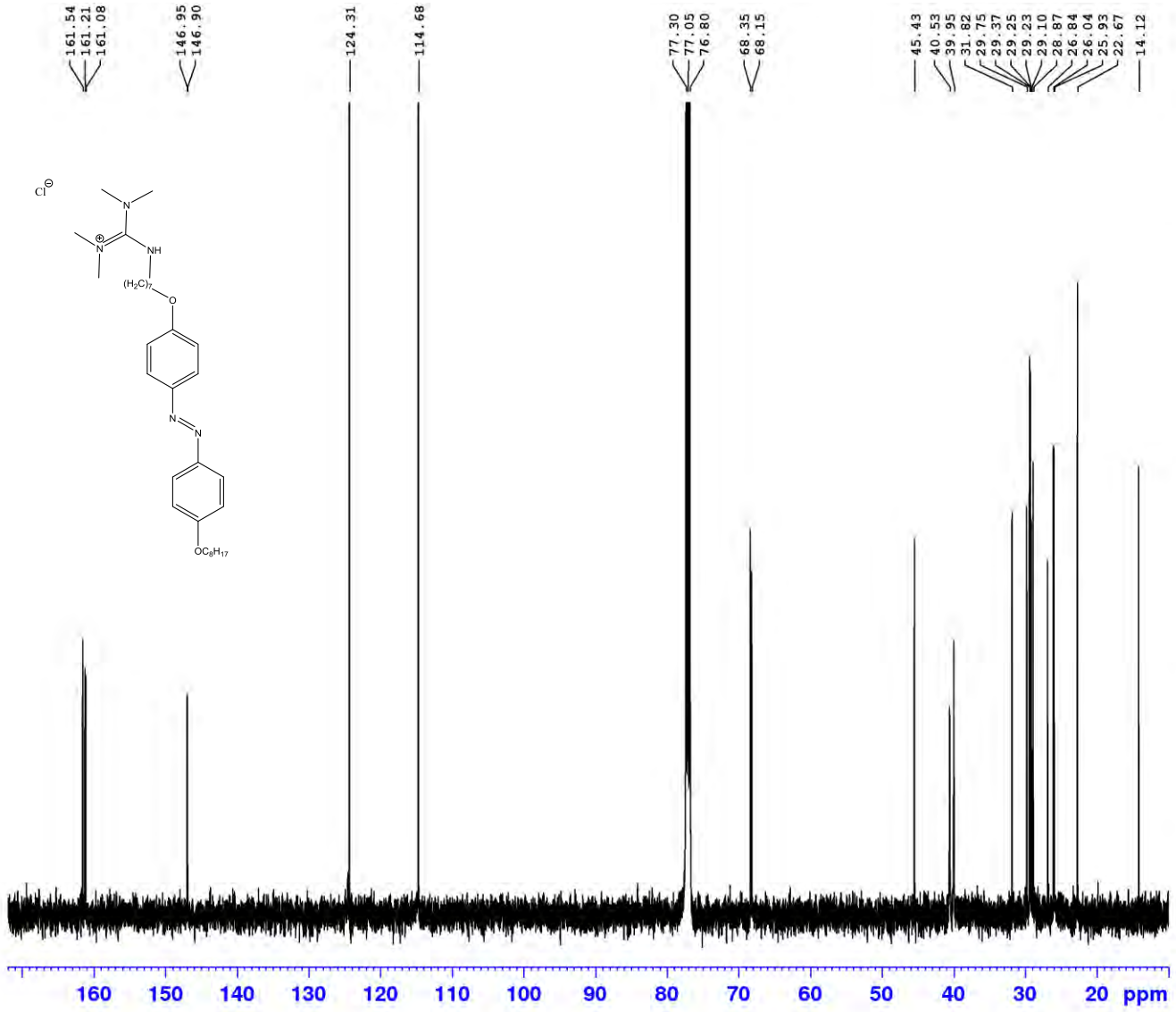
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste








```
Current Data Parameters
NAME                 0ct31-2012
EXPNO                       230
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20121031
Time                      19.42
INSTRUM                   spect
PROBHD    5 mm QNP 1H/13
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                   5175.983 Hz
FIDRES                0.078979 Hz
AQ                    6.3307776 sec
RG                        203.2
DW                       96.600 usec
DE                        8.00 usec
TE                       300.0 K
D1                    1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       10.40 usec
PL1                      -6.00 dB
SFO1                250.1315447 MHz

F2 - Processing parameters
SI                       65536
SF                  250.1300030 MHz
WDW                         EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```

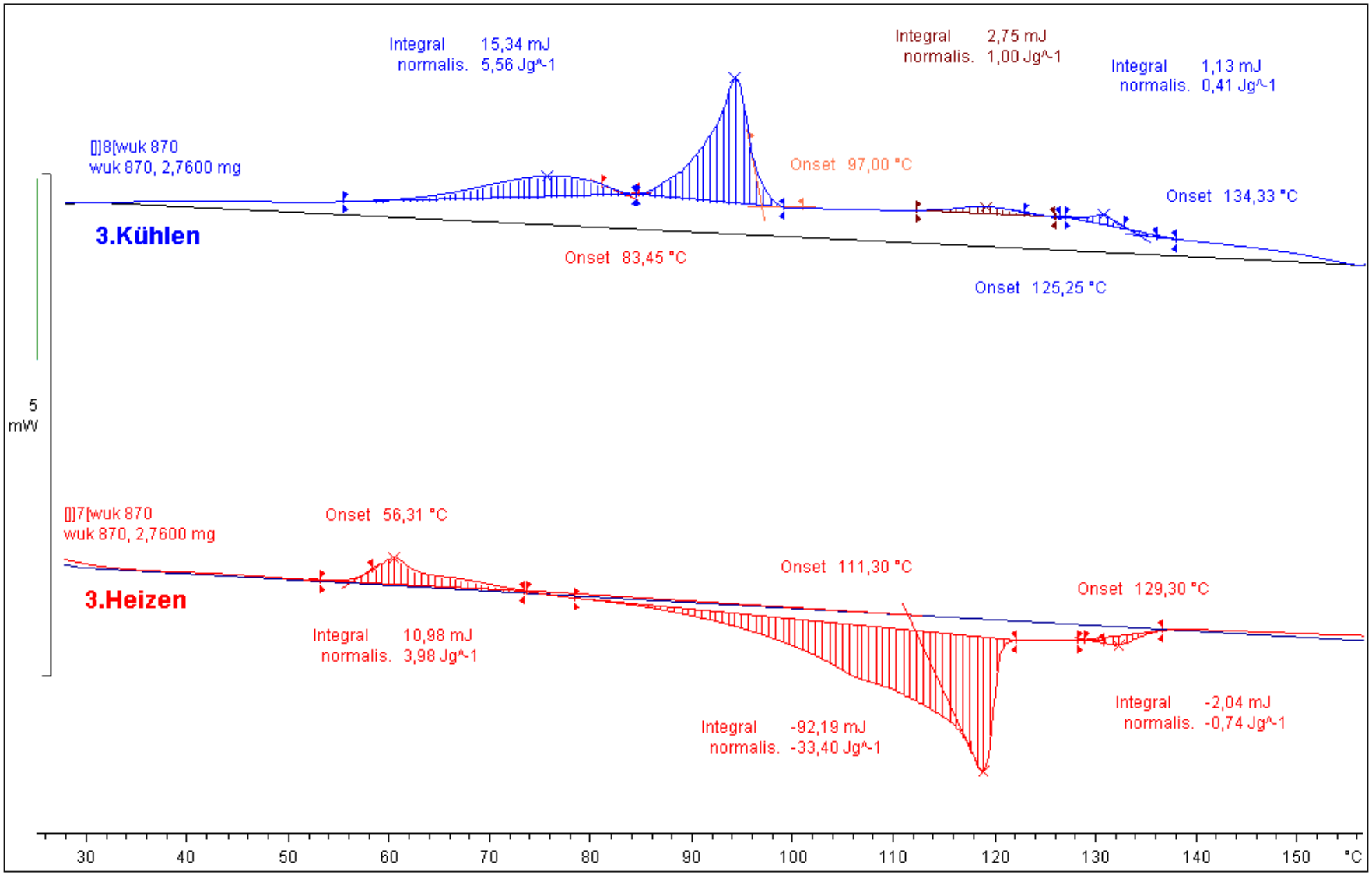


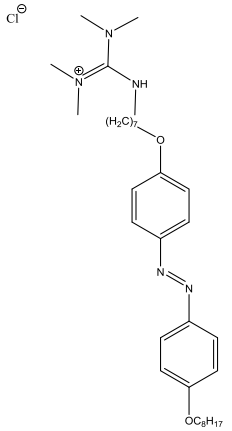

```
Current Data Parameters
NAME          Sep19-2014
EXPNO                 51
PROCNO                 1

F2 - Acquisition Parameters
Date_          20140919
Time              13.56
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                2048
DS                   4
SWH          32894.738 Hz
FIDRES        0.501934 Hz
AQ            0.9961472 sec
RG                2890
DW              15.200 usec
DE              10.00 usec
TE               296.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                10.20 usec
PL1                1.50 dB
PL1W        51.74793243 W
SFO1       125.7761482 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2             100.00 usec
PL2                1.00 dB
PL12              19.99 dB
PL13              21.00 dB
PL2W        19.75309753 W
PL12W        0.24925002 W
PL13W        0.19753097 W
SFO2       500.1550006 MHz

F2 - Processing parameters
SI                 32768
SF         125.7635720 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

^exo

wuk 870 3x integriert

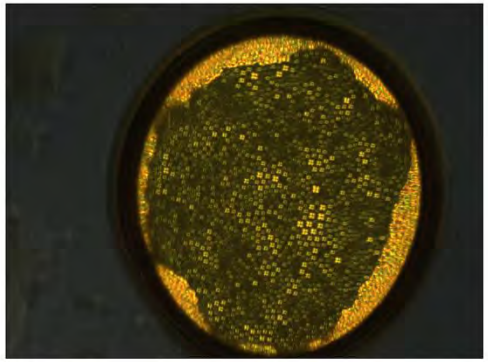
18.09.2014 15:41:20



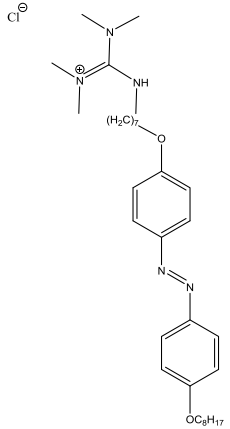


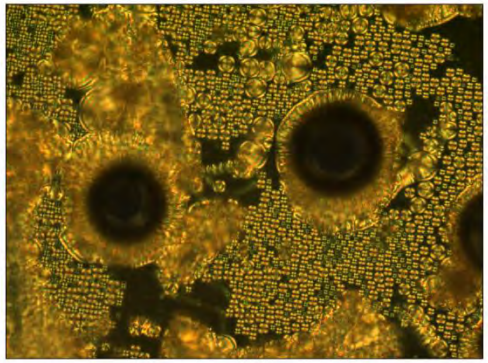
Uni Stuttgart - AK Laschat: Wuckert

METTLER TOLEDO STAR^{e} SW 7.01

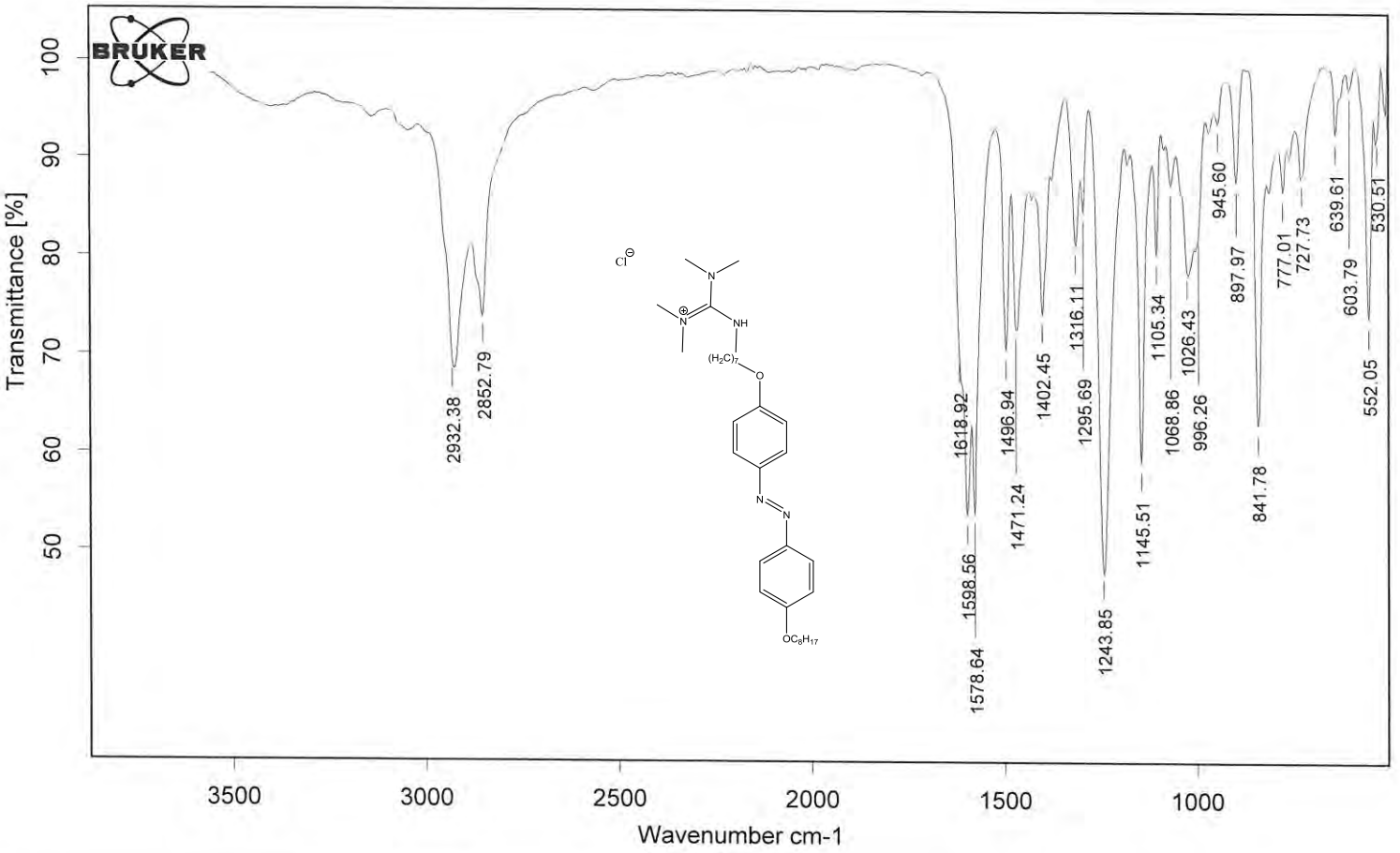


Bildname: wuk 870.4.4
Bildkommentar: Kühlen von 148° (Schmelze) mit 1°/min
bei 140°
200x





Bildname: wuk 870.trock.1
Bildkommentar: Kühlen mit 5°/min von ca. 145° (I)
bei 120°
200x



D:\IR-DATEN\Wegner\8sp7 870.0	Wuckert/8sp7 870	fest	15/01/2014

Druckprot

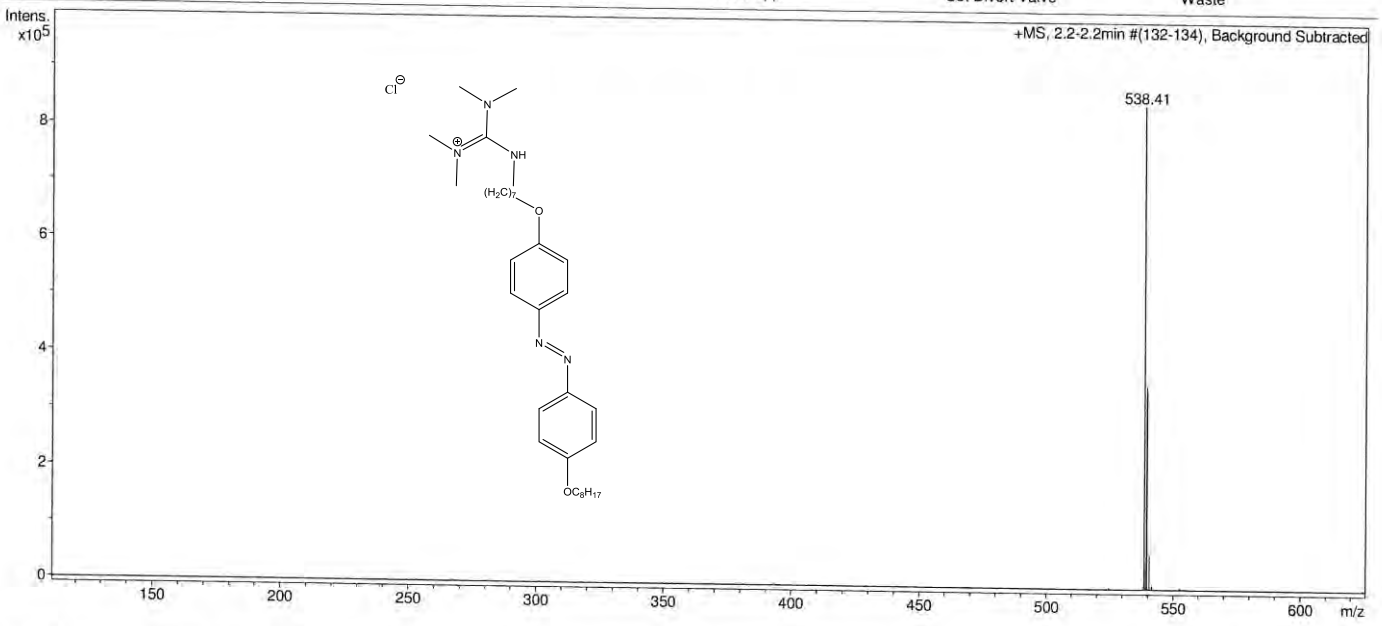
Massenspektrometrie - Universität Stuttgart

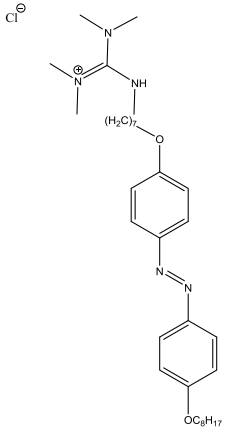
Analysis Info

Analysis Name	Laschat-Wuckert WUK 870_2_01_18757.d	Acquisition Date	22.11.2012 13:57:54
Method	loop-tune-low.m		
Sample Name	Laschat-Wuckert WUK 870	Operator	wo/tri
Comment		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





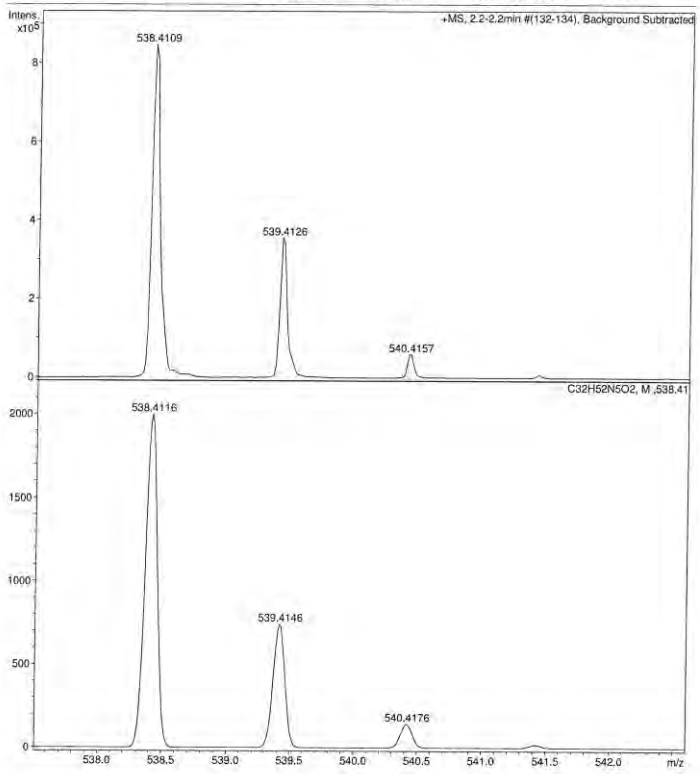
Massenspektrometrie - Universität Stuttgart

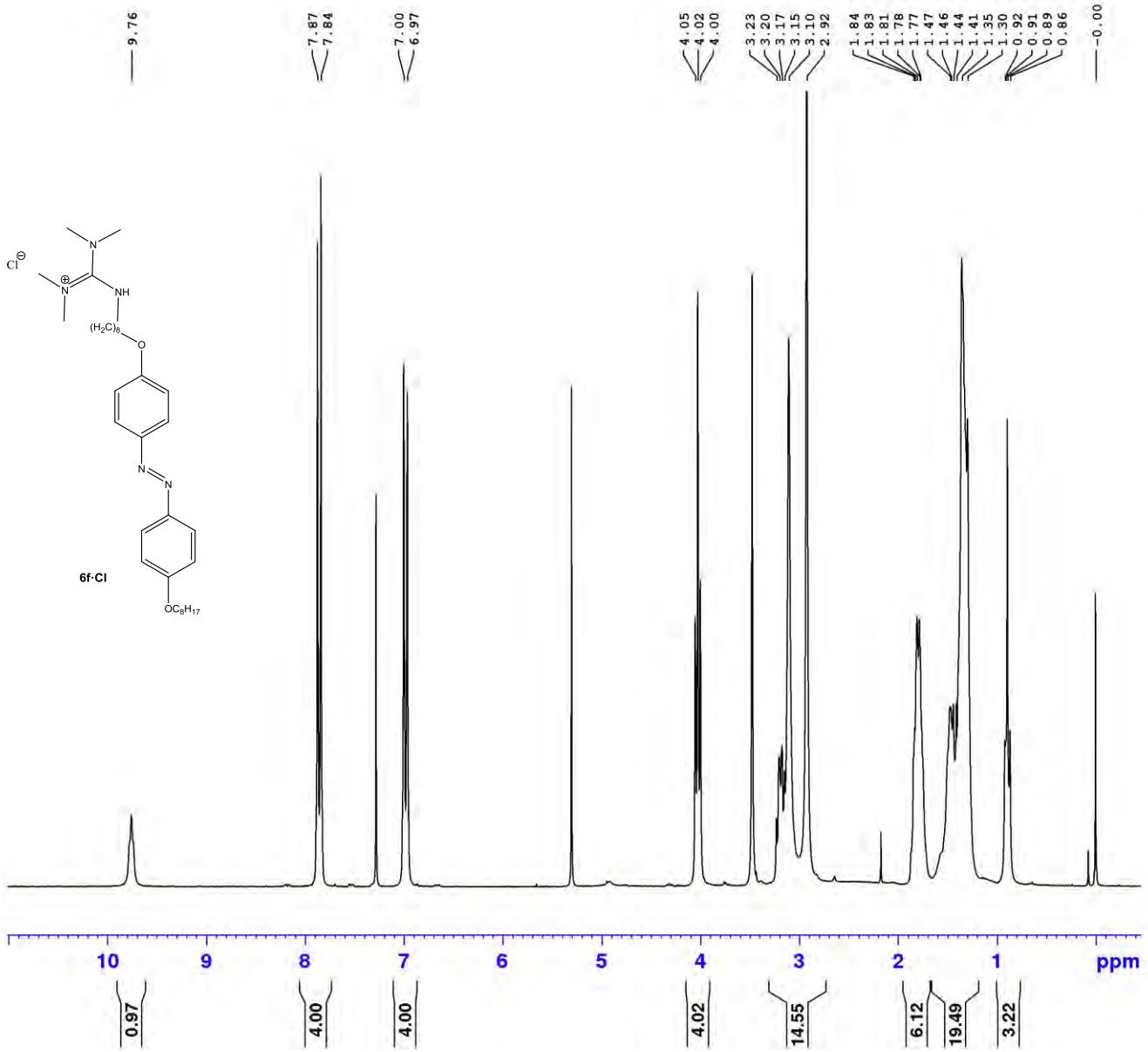
Analysis Info

Analysis Name	Laschat-Wuckert WUK 870_2_01_18757.d	Acquisition Date	22.11.2012 13:57:54
Method	loop-tune-low.m	Operator	wo/tri
Sample Name	Laschat-Wuckert WUK 870	Instrument	micrOTOF-Q 43
Comment			

Acquisition Parameter

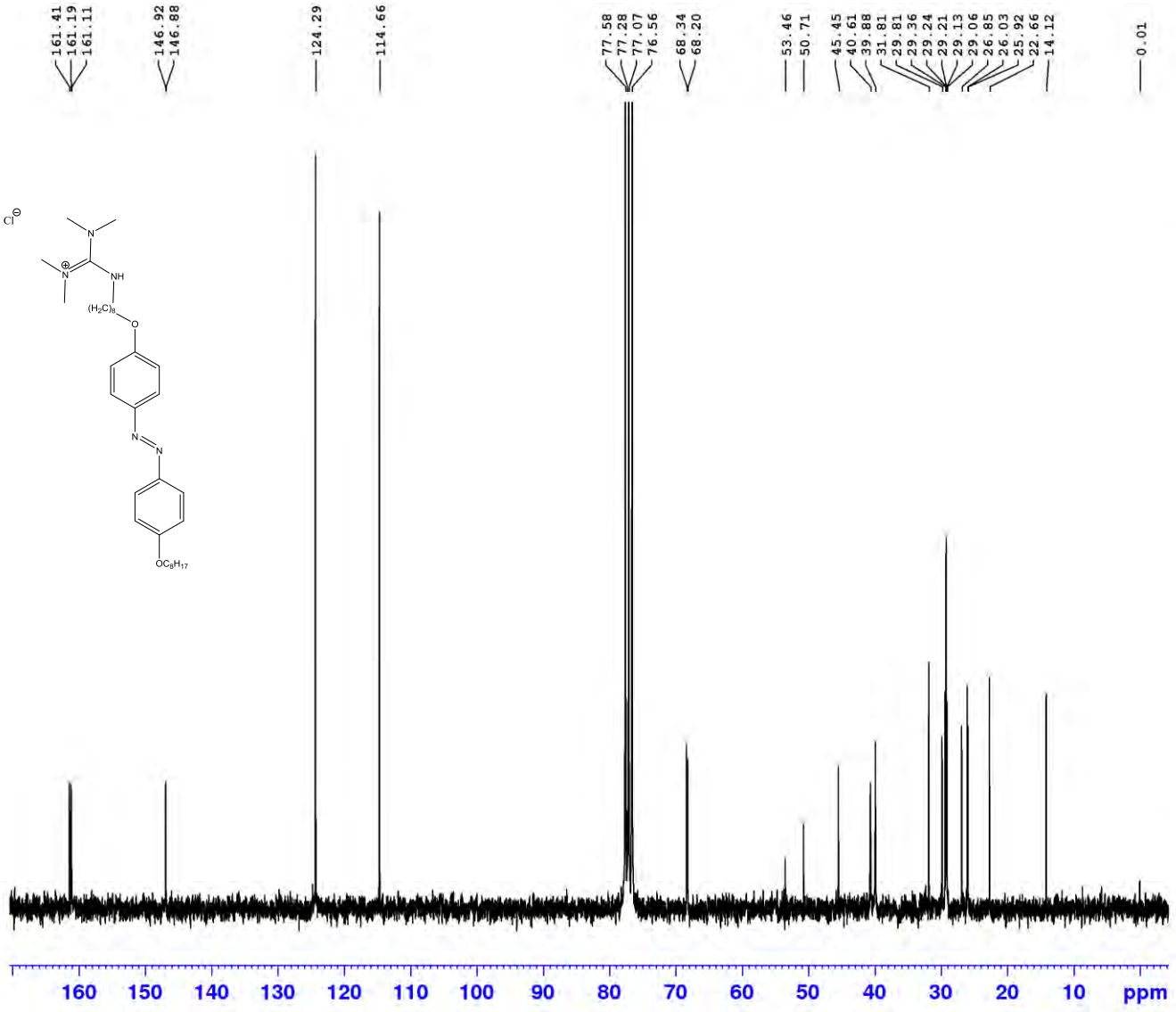
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.8 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Waste





6f·Cl

```
Current Data Parameters
NAME                 Apr16-2013
EXPNO                        80
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20130416
Time                      10.39
INSTRUM                   spect
PROBHD    5 mm QNP 1H/13
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           32
DS                            2
SWH                    5175.983 Hz
FIDRES                 0.078979 Hz
AQ                     6.3307776 sec
RG                         228.1
DW                        96.600 usec
DE                         8.00 usec
TE                        300.0 K
D1                     1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                         1H
P1                        10.40 usec
PL1                       -6.00 dB
SFO1                250.1315447 MHz

F2 - Processing parameters
SI                        65536
SF                 250.1300025 MHz
WDW                          EM
SSB                0
LB                         0.30 Hz
GB                 0
PC                         1.00
```

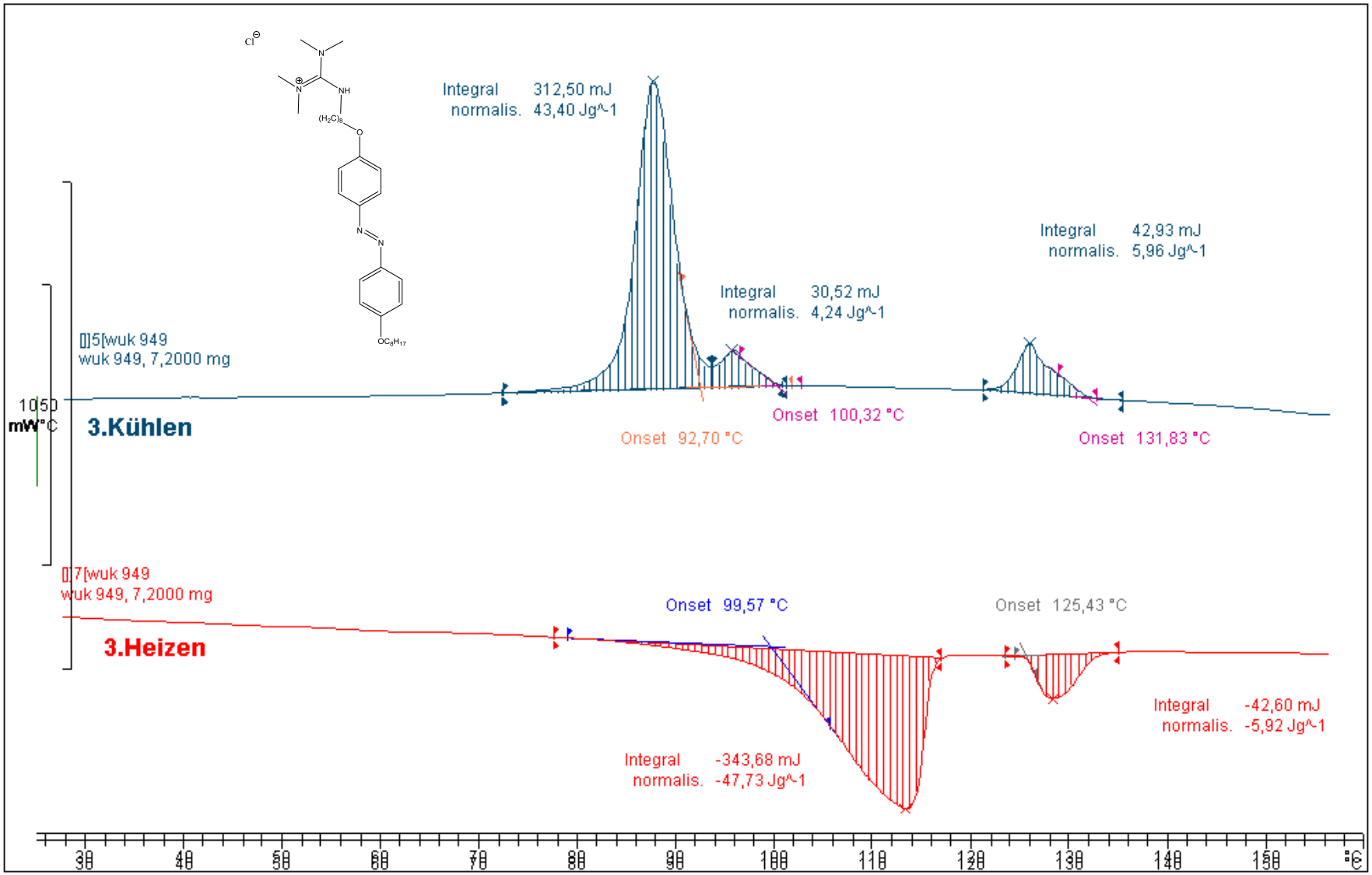



```
Current Data Parameters
NAME                  Apr16-2013
EXPNO                         81
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20130416
Time                       11.52
INSTRUM                    spect
PROBHD   5 mm QNP 1H/13
PULPROG                  zgpg30
TD                          65536
SOLVENT                     CDC13
NS                           1024
DS                              4
SWH                  15060.241 Hz
FIDRES                0.229801 Hz
AQ                    2.1757953 sec
RG                          13004
DW                         33.200 usec
DE                          8.00 usec
TE                         300.0 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                         13C
P1                         11.70 usec
PL1          0 dB
SFO1                62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                         1H
PCPD2                    100.00 usec
PL2                       -6.00 dB
PL12                      18.50 dB
PL13                      15.00 dB
SFO2                250.1310005 MHz

F2 - Processing parameters
SI                           32768
SF                  62.8952390 MHz
WDW                             EM
SSB          0
LB                         1.00 Hz
GB           0
PC                         1.40
```

^exo

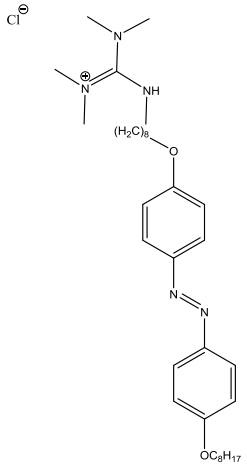
wuk 949 3x integriert

18.09.2014 15:44:43

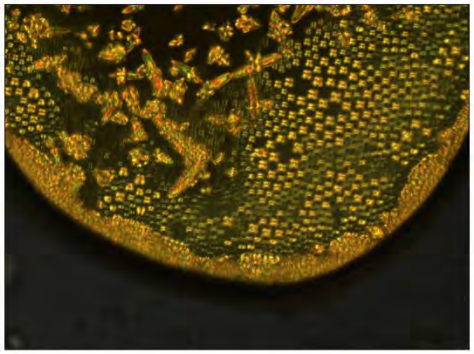


Uni Stuttgart - AK Laschat: Wuckert

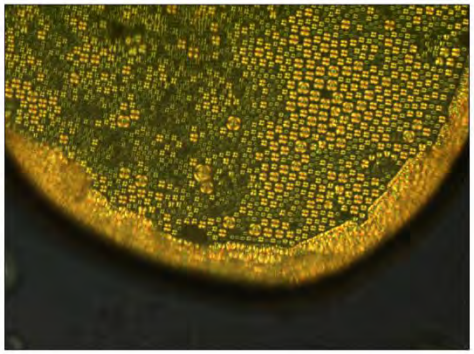
METTLER TOLEDO STAR^{e} SW 7.01



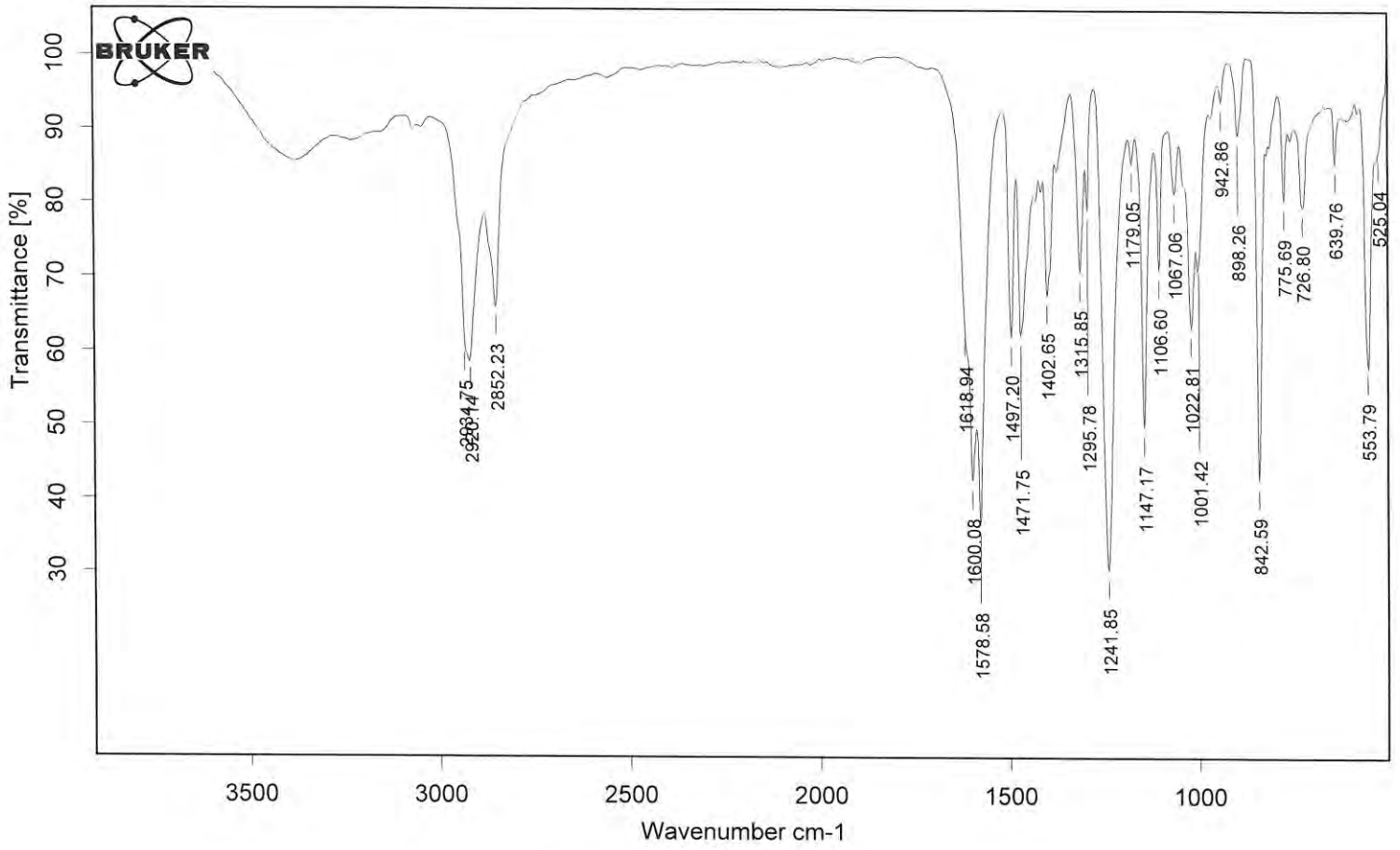
8 Sp 8 (wuk 857)

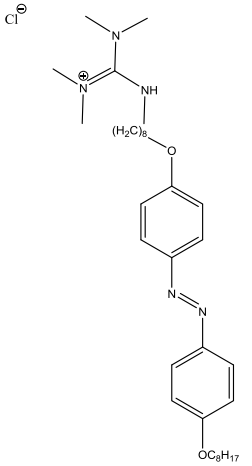


Bildname: wuk 857A.2
Bildkommentar: Kühlen von der Schmelze (133°) mit unterschiedl. Kühlrate
bei 130°
200x



Bildname: wuk 857A.3
Bildkommentar: Kühlen von der Schmelze (133°) mit unterschiedl. Kühlrate
bei 129°
200x





D:\IR-DATEN\Wegner\8sp8 949.0	Wuckert/8sp8 949	fest	15/01/2014

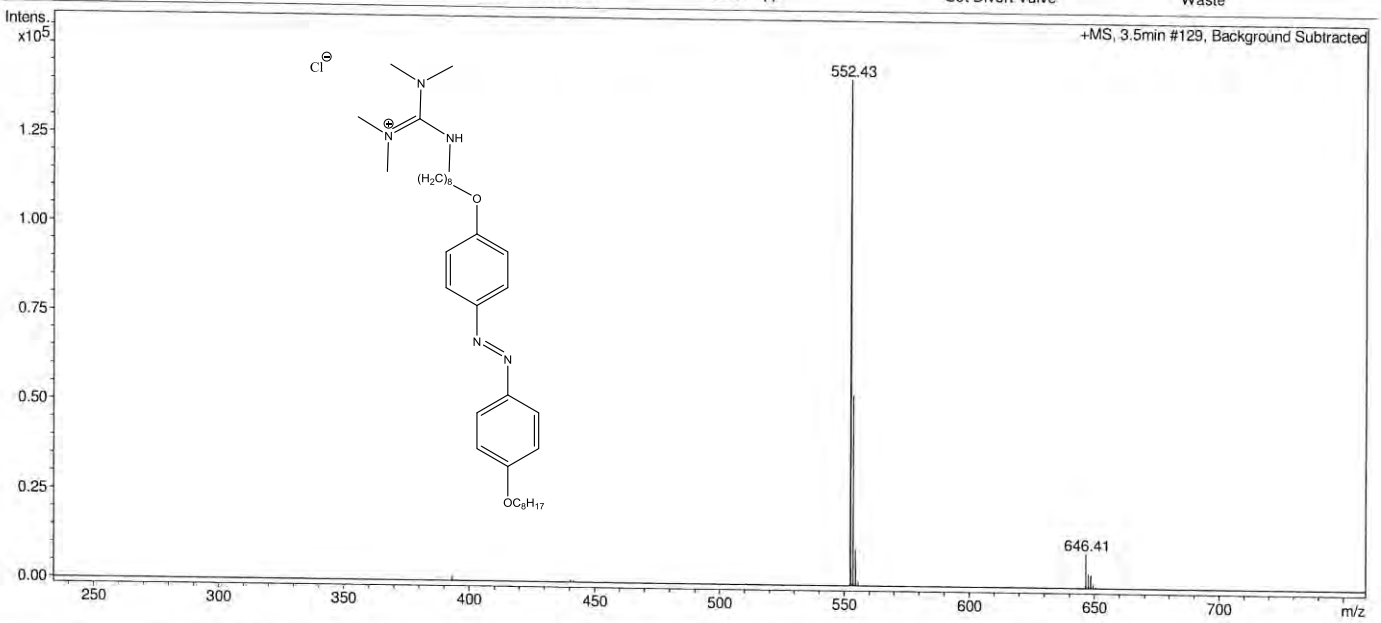
Massenspektrometrie - Universität Stuttgart

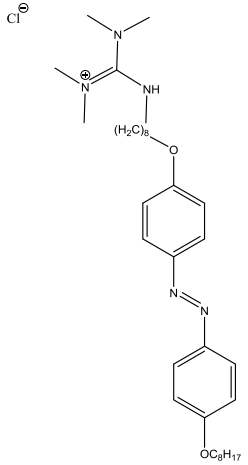
Analysis Info

Analysis Name	Laschat-Wuckert WUK 857A_2_01_18468.d	Acquisition Date	23.10.2012 08:42:27
Method	test-withloop.m		
Sample Name	Laschat-Wuckert WUK 857A	Operator	wo/tri
Comment		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	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	580.0 Vpp	Set Divert Valve	Waste





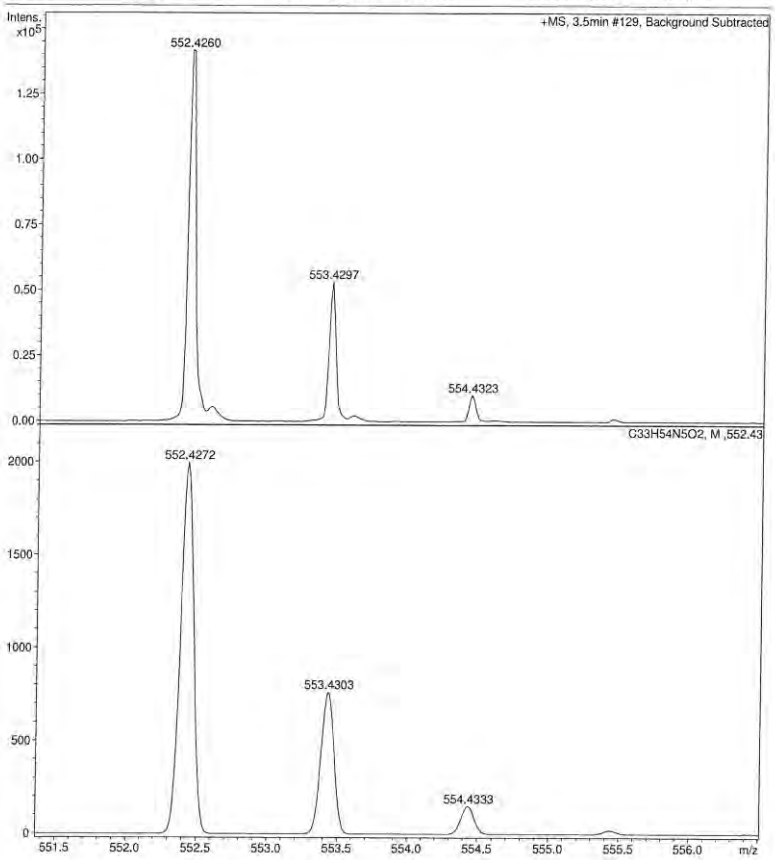
Massenspektrometrie - Universität Stuttgart

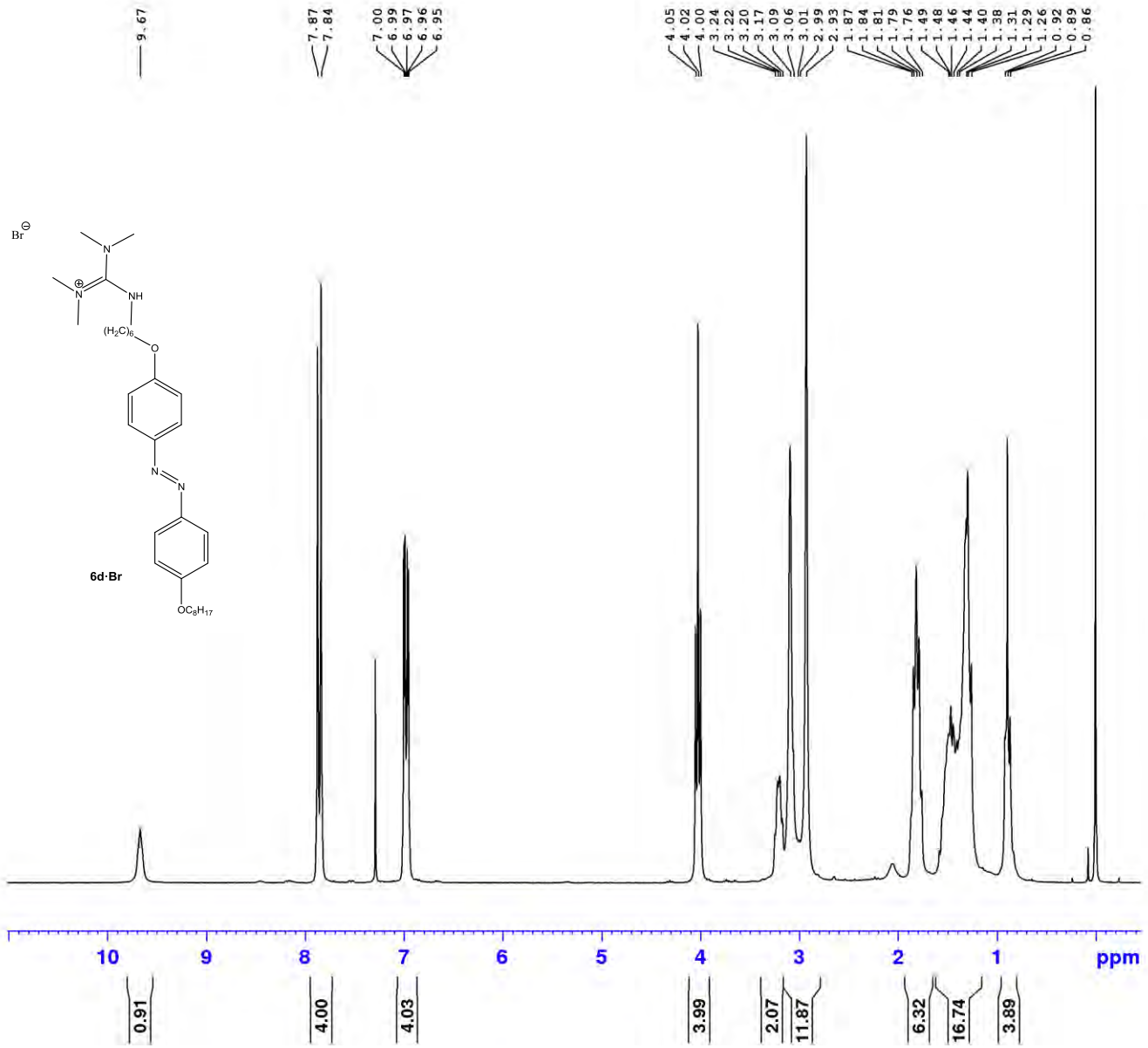
Analysis Info

Analysis Name	Laschat-Wuckert WUK 857A_2_01_18468.d	Acquisition Date	23.10.2012 08:42:27
Method	test-withloop.m	Operator	wo/tri
Sample Name	Laschat-Wuckert WUK 857A	Instrument	micrOTOF-Q 43
Comment			

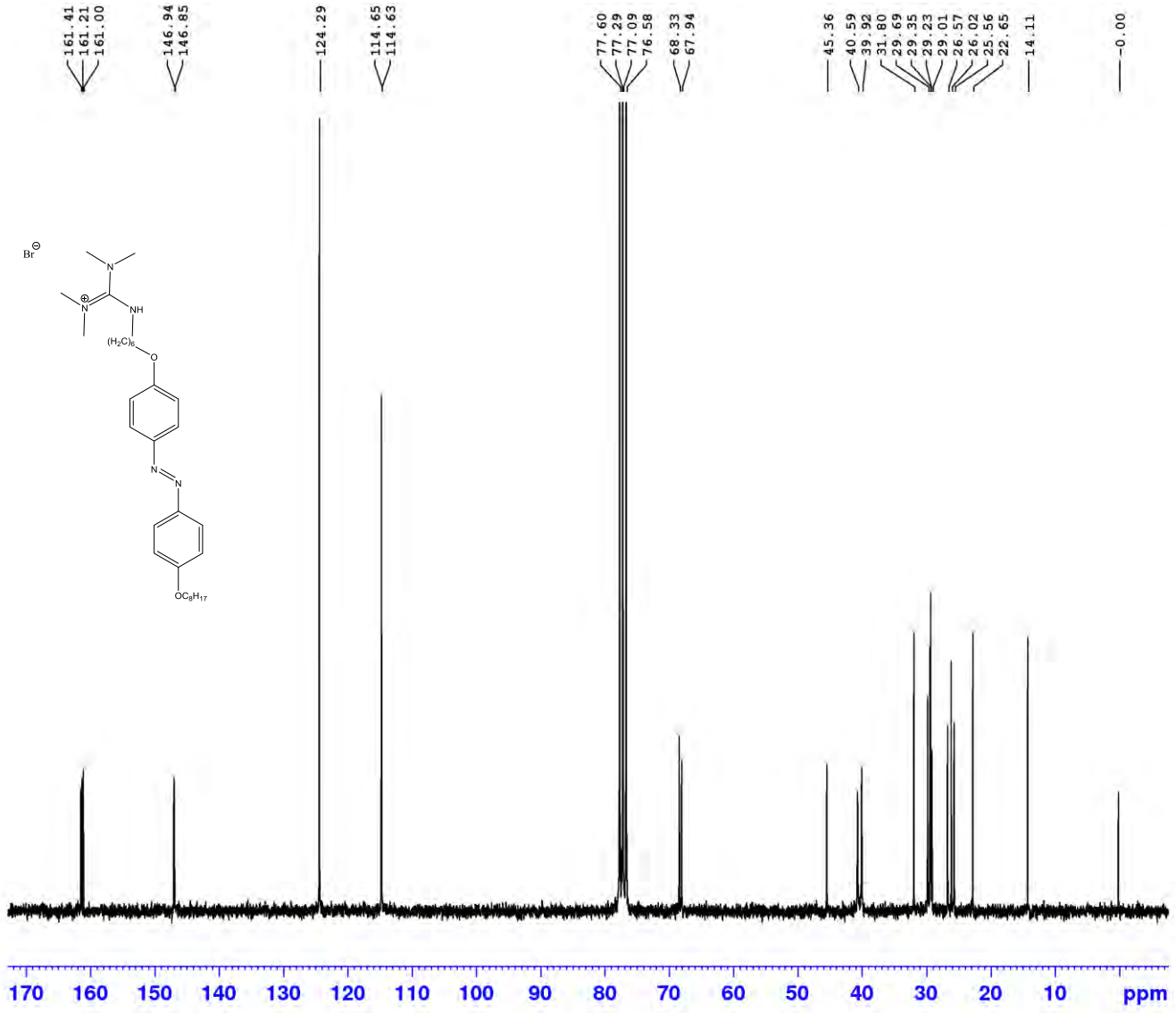
Acquisition Parameter

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	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	580.0 Vpp	Set Divert Valve	Waste



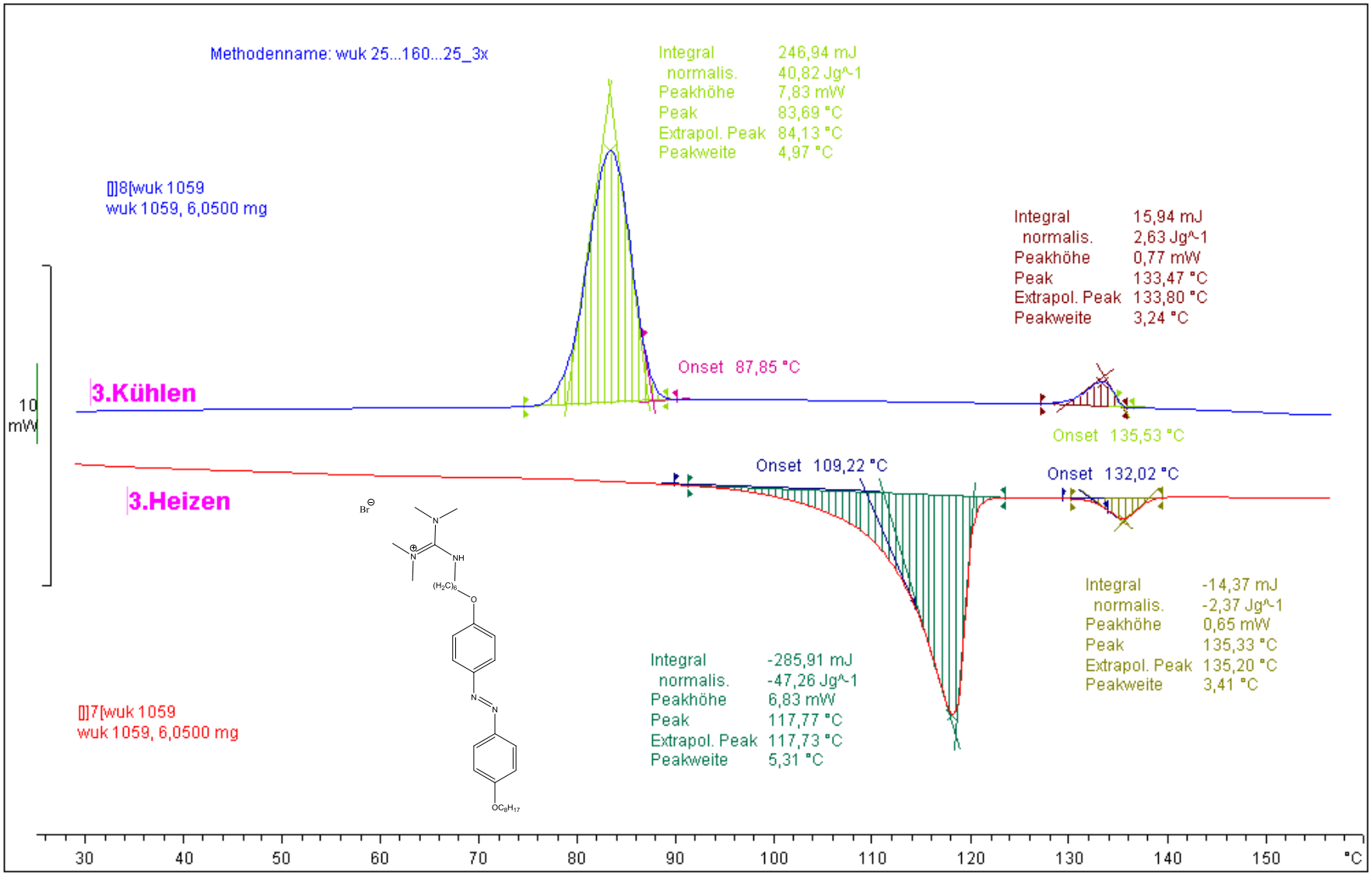



```
Current Data Parameters
NAME                  Jan28-2014
EXPNO                         80
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20140128
Time                       19.45
INSTRUM                    spect
PROBHD    5 mm QNP 1H/13
PULPROG                     zg30
TD                         65536
SOLVENT                    CDCl3
NS                            64
DS                             2
SWH                     5175.983 Hz
FIDRES                  0.078979 Hz
AQ                    6.3307776 sec
RG                         143.7
DW                        96.600 usec
DE                         8.00 usec
TE                        300.0 K
D1                    1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                        10.40 usec
PL1                       -6.00 dB
SFO1                250.1315447 MHz

F2 - Processing parameters
SI                         65536
SF                  250.1300009 MHz
WDW                           EM
SSB                0
LB                         0.30 Hz
GB                 0
PC                         1.00
```



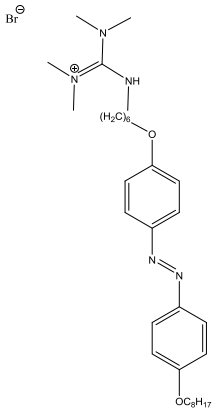

```
Current Data Parameters
NAME                  Jan28-2014
EXPNO                         81
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20140128
Time                       22.10
INSTRUM                    spect
PROBHD   5 mm QNP 1H/13
PULPROG                  zgpg30
TD                          65536
SOLVENT                     CDC13
NS                           2048
DS                              4
SWH                  15060.241 Hz
FIDRES                0.229801 Hz
AQ                    2.1757953 sec
RG                       2896.3
DW                        33.200 usec
DE                         8.00 usec
TE                        300.0 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                         13C
P1                         11.70 usec
PL1       0 dB
SFO1                62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                         1H
PCPD2                    100.00 usec
PL2                       -6.00 dB
PL12                      18.50 dB
PL13                      15.00 dB
SFO2                250.1310005 MHz

F2 - Processing parameters
SI                           32768
SF                   62.8952344 MHz
WDW                             EM
SSB       0
LB                         1.00 Hz
GB        0
PC                         1.40
```

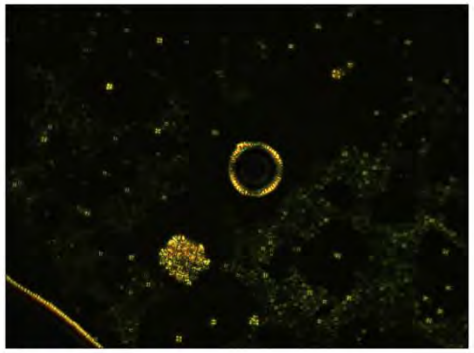
^exo wuk 1059_3.Lauf 18.09.2014 15:45:41



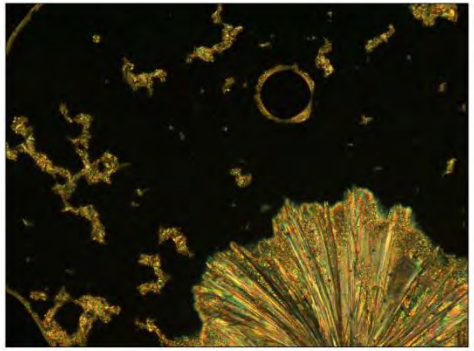
Uni Stuttgart - AK Laschat: Wuckert METTLER TOLEDO STAR^{e} SW 7.01

8 Sp 6 Bromid (wuk 1059)

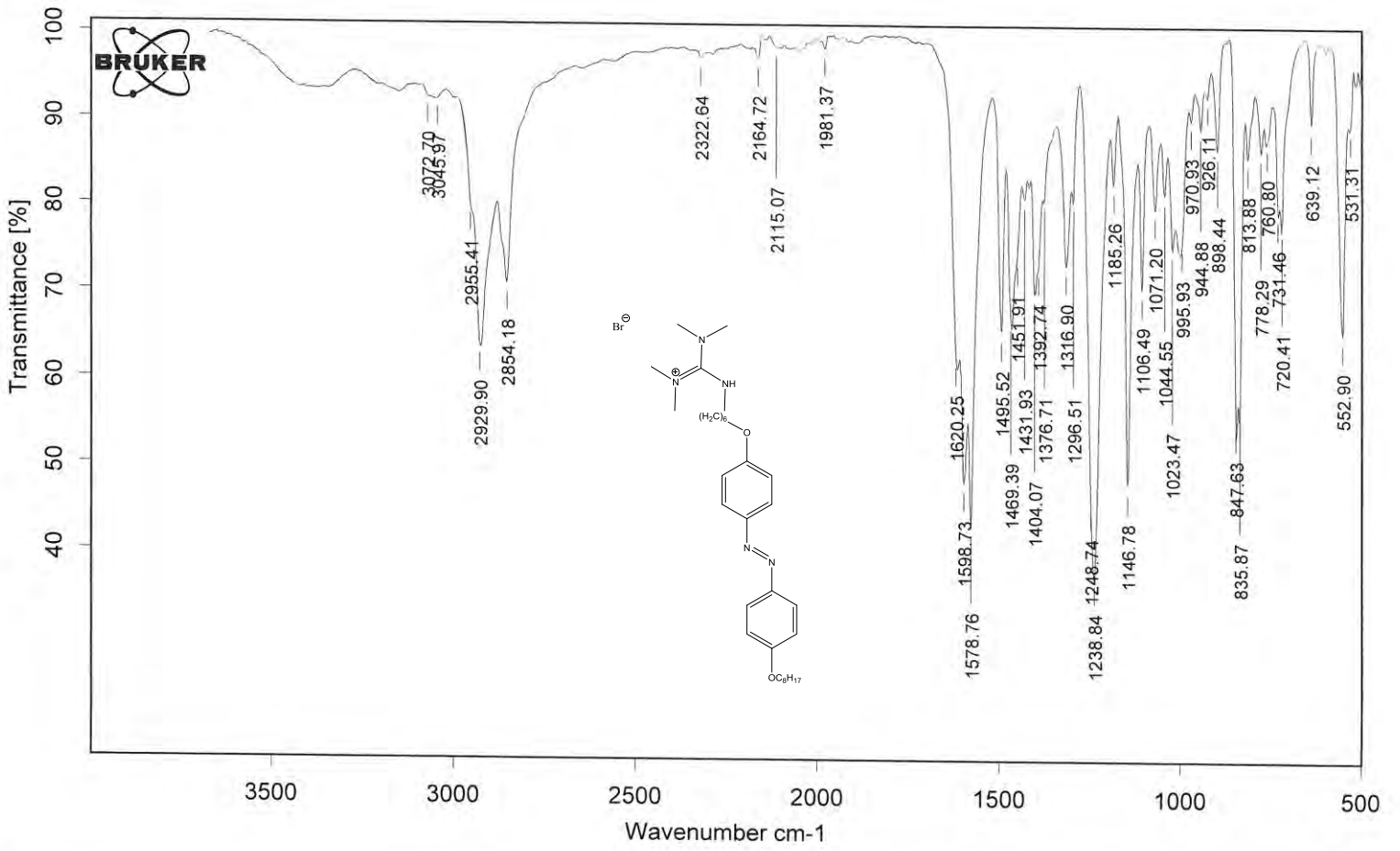




Bildname: wuk 1059.2
Bildkommentar: Kühlen von I bei 140° mit 1°/min
aufgenom. bei 132°
200x



Bildname: 1059.5
Bildkommentar: Kühlen von 142° - I mit 10°/min
die ersten Text. bei ca. 139°
89.5° Cr
200x



D:\IR-Daten\Wegner\1059.0	Wuckert/1059	fest	05/02/2014

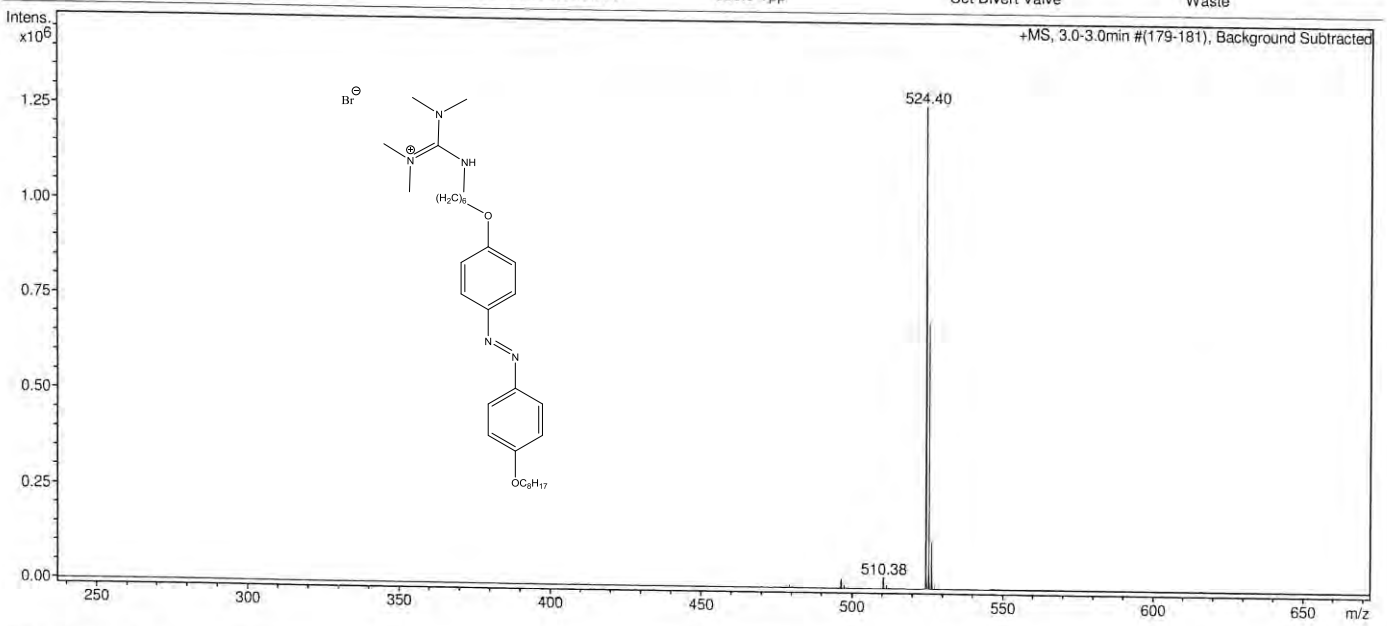
Massenspektrometrie - Universität Stuttgart

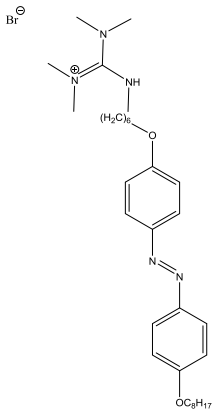
Analysis Info

Analysis Name	Laschat-Wuckert WUK 1059_10_01_23018.d	Acquisition Date	06.02.2014 09:39:23
Method	test-withloop.m		
Sample Name	Laschat-Wuckert WUK 1059	Operator	wo/tri
Comment		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





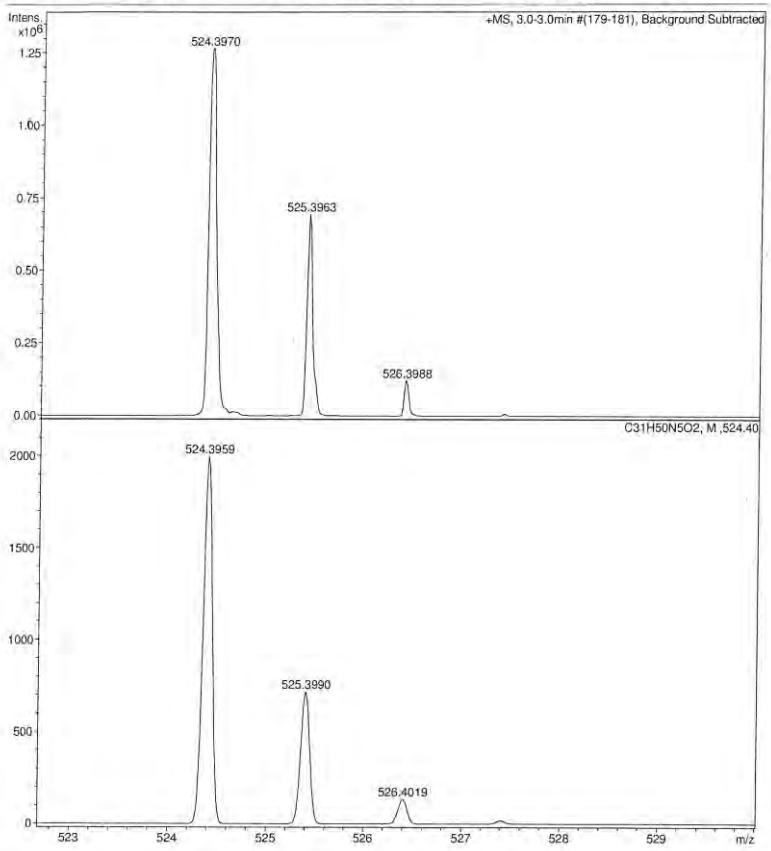
Massenspektrometrie - Universität Stuttgart

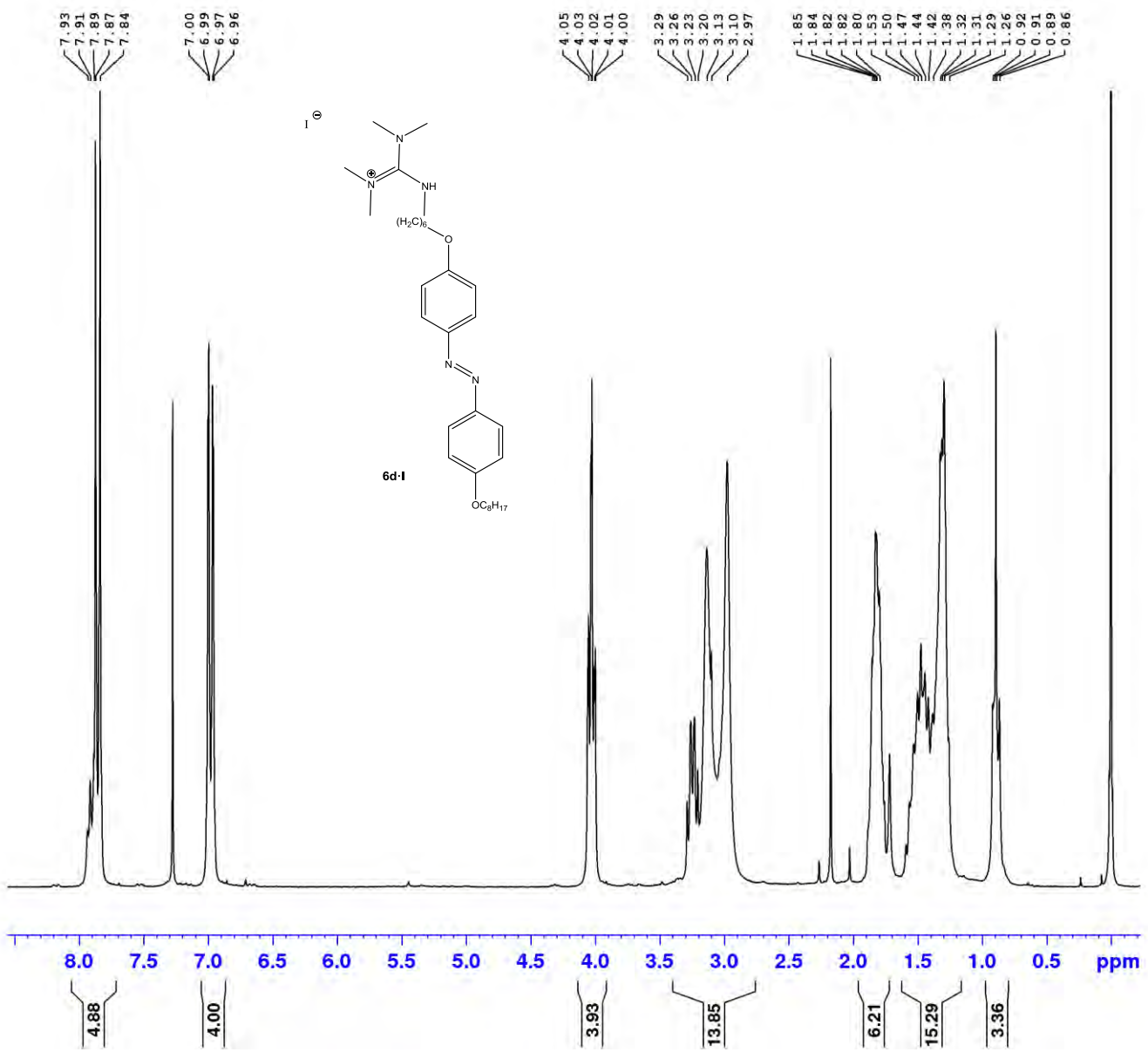
Analysis Info

Analysis Name	Laschat-Wuckert WUK 1059_10_01_23018.d	Acquisition Date	06.02.2014 09:39:23
Method	test-withloop.m	Operator	wo/tri
Sample Name	Laschat-Wuckert WUK 1059	Instrument	micrOTOF-Q 43
Comment			

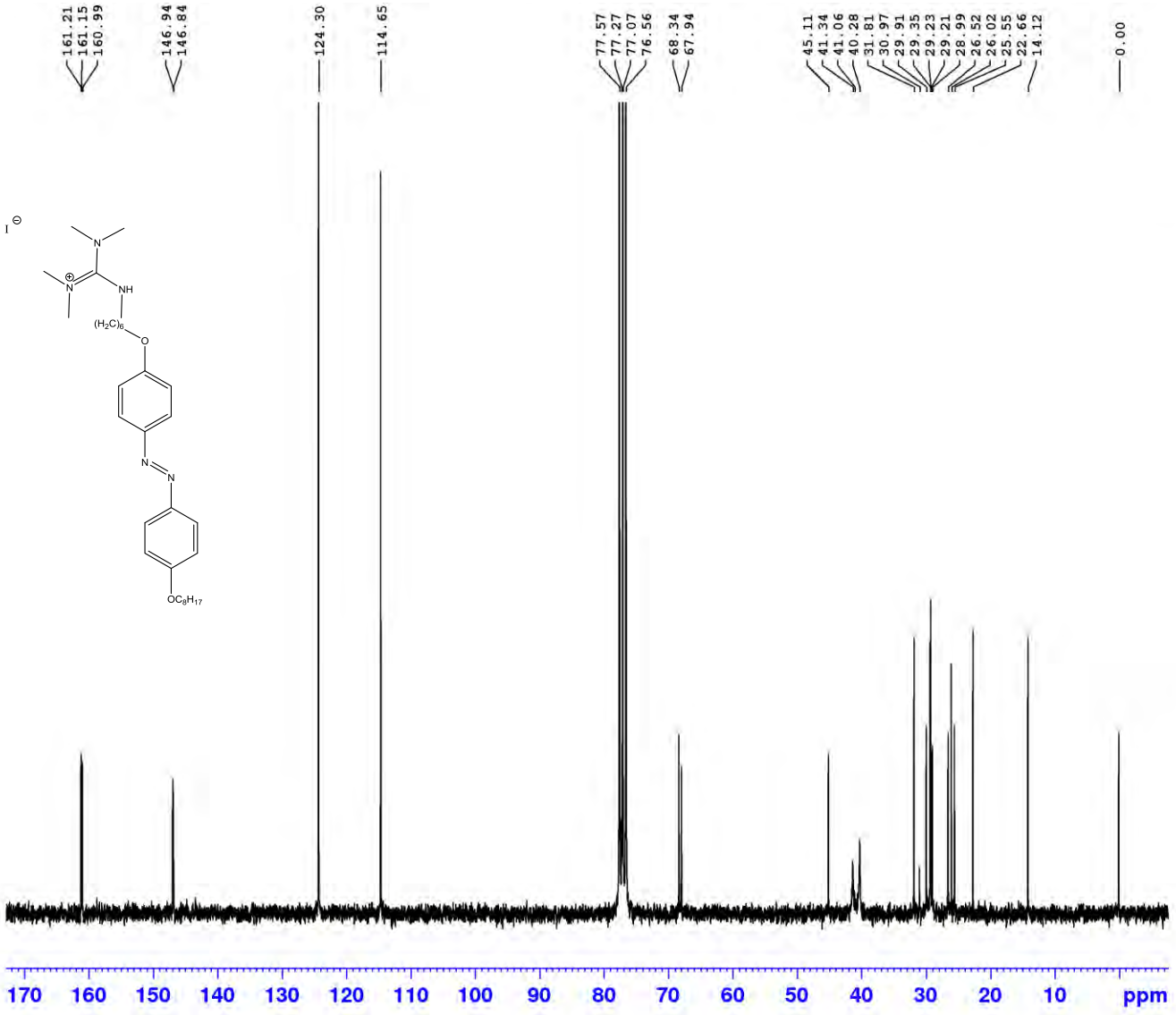
Acquisition Parameter

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



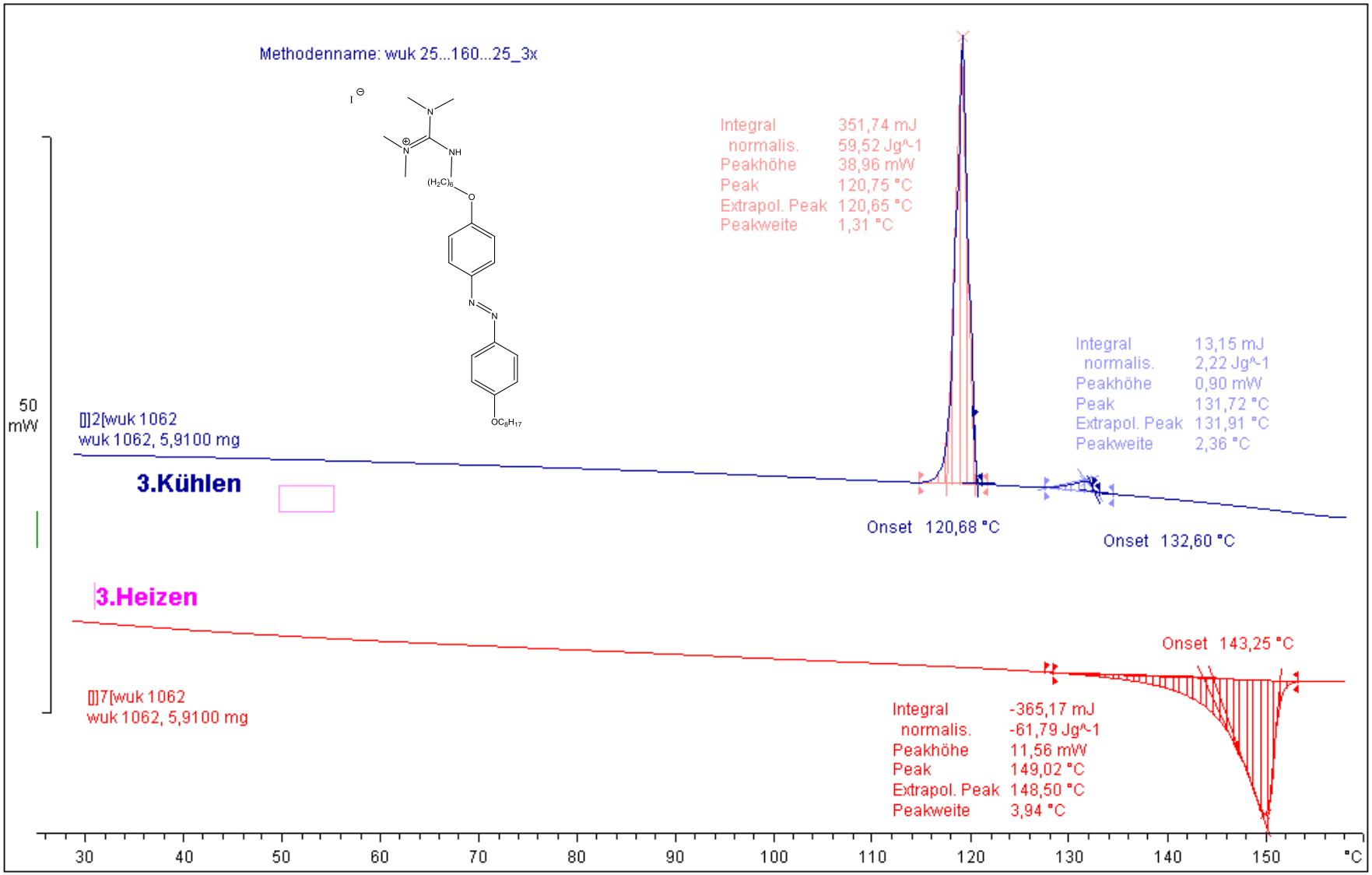



```
Current Data Parameters
NAME                  Jan31-2014
EXPNO                        390
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20140201
Time                        1.48
INSTRUM                    spect
PROBHD   5 mm QNP 1H/13
PULPROG                     zg30
TD                         65536
SOLVENT                    CDCl3
NS                            64
DS                             2
SWH                     5175.983 Hz
FIDRES                  0.078979 Hz
AQ                    6.3307776 sec
RG                         228.1
DW                        96.600 usec
DE                         8.00 usec
TE                        300.0 K
D1                    1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                        10.40 usec
PL1                       -6.00 dB
SFO1                250.1315447 MHz

F2 - Processing parameters
SI                         65536
SF                  250.1300042 MHz
WDW                           EM
SSB                0
LB                        0.30 Hz
GB                 0
PC                        1.00
```

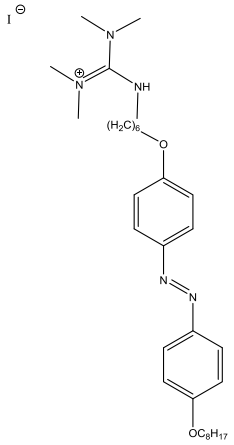



```
Current Data Parameters
NAME                  Jan31-2014
EXPNO                        391
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20140201
Time                        5.26
INSTRUM                    spect
PROBHD   5 mm QNP 1H/13
PULPROG                  zgpg30
TD                          65536
SOLVENT                     CDC13
NS                           3072
DS                              4
SWH                  15060.241 Hz
FIDRES                0.229801 Hz
AQ                    2.1757953 sec
RG                       2896.3
DW                        33.200 usec
DE                         8.00 usec
TE                        300.0 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                         13C
P1                         11.70 usec
PL1        0 dB
SFO1                62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                         1H
PCPD2                    100.00 usec
PL2                       -6.00 dB
PL12                      18.50 dB
PL13                      15.00 dB
SFO2                250.1310005 MHz

F2 - Processing parameters
SI                           32768
SF                  62.8952399 MHz
WDW                             EM
SSB        0
LB                         1.00 Hz
GB         0
PC                         1.40
```

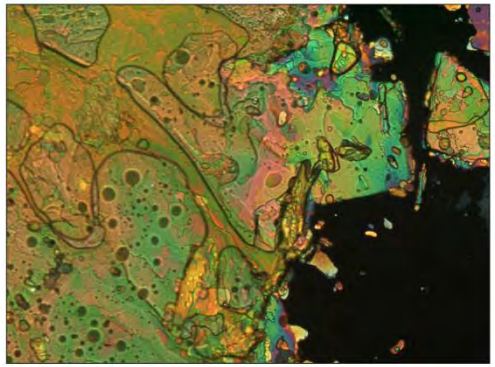
^exo wuk 1062_3.Lauf 18.09.2014 15:47:48



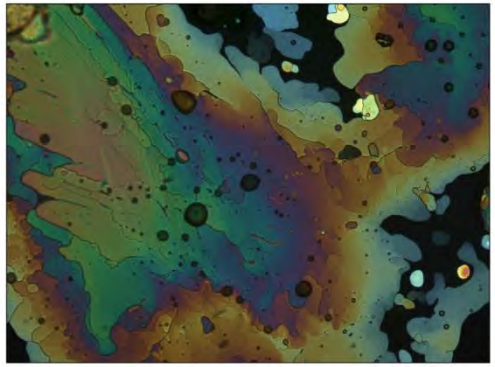
Uni Stuttgart - AK Laschat: Wuckert METTLER TOLEDO STAR^{e} SW 7.01



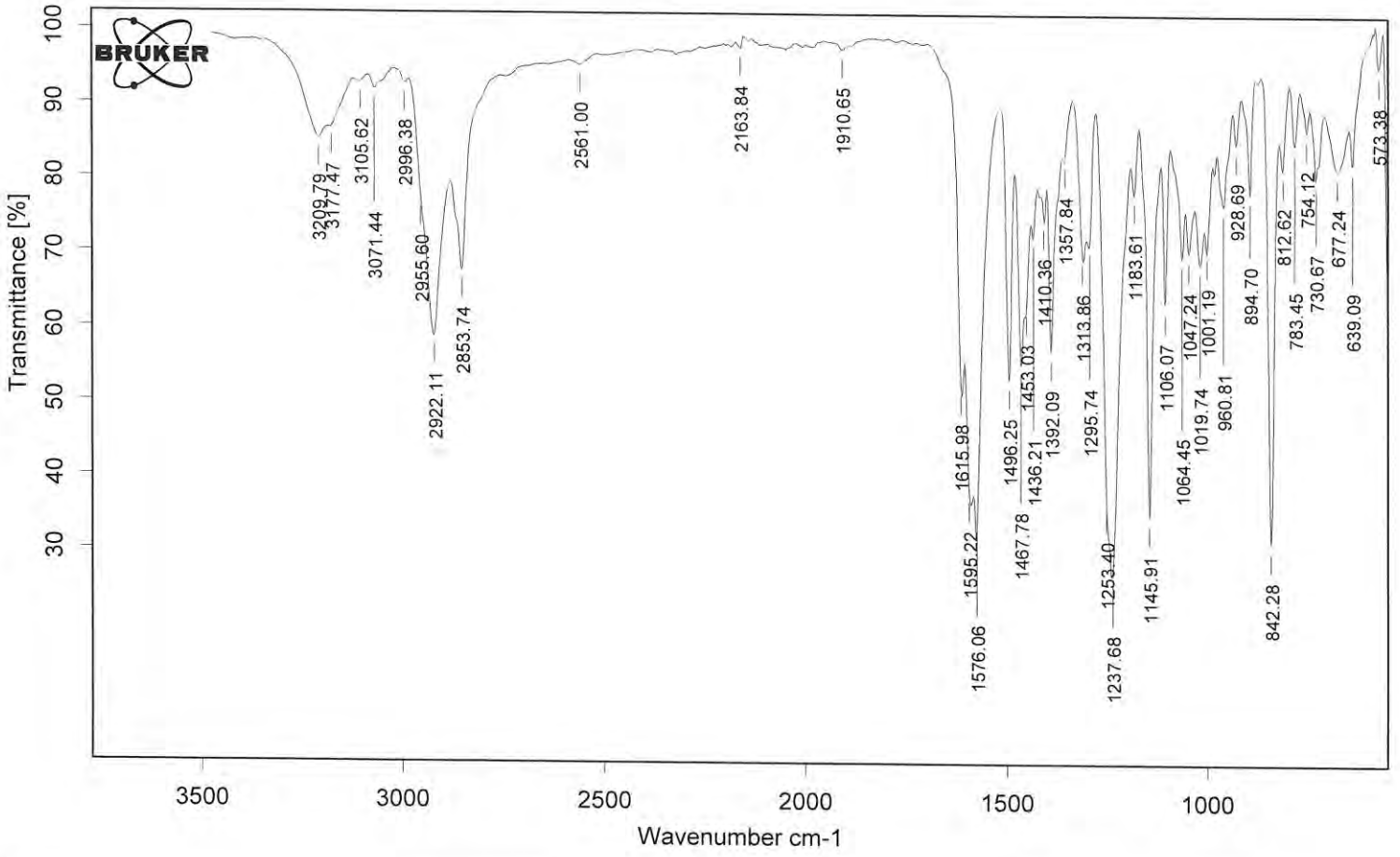
8 Sp 6 Jodid (wuk 1062)

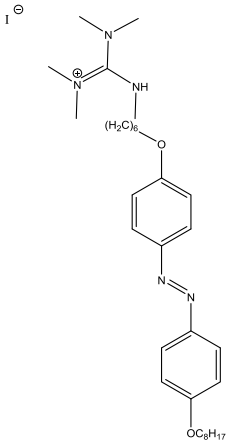


Bildname: wuk 1062.1
Bildkommentar: Kühlen von 153° - I mit 1°/min
aufgen. bei 145°
Cr schwimmen in Flüssigkeit
100x



Bildname: wuik 1062.2
Bildkommentar: Kühlen von 153° - I mit 1°/min
aufgen. bei 142°
Cr schwimmen in Flüssigkeit
100x





D:\IR-DATEN\twiehaus\1062.0	Wuckert/1062	fest	31/01/2014

Unclear

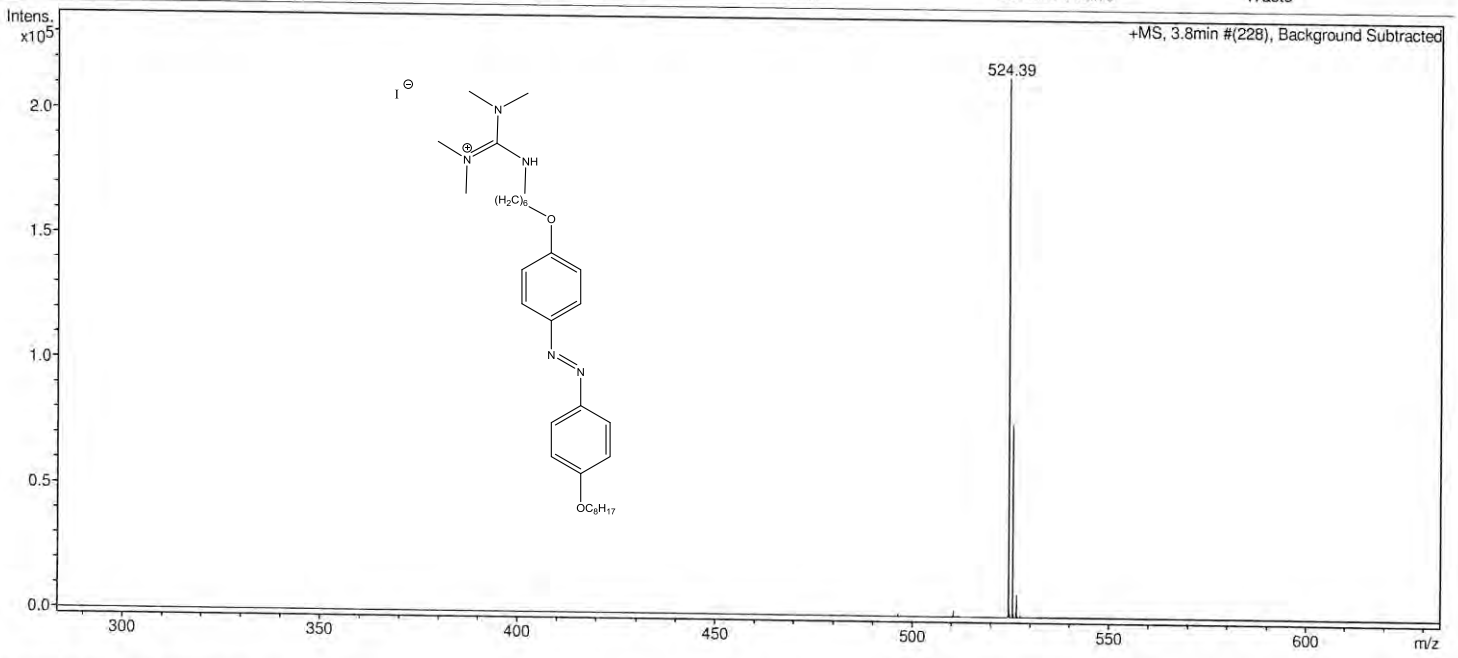
Massenspektrometrie - Universität Stuttgart

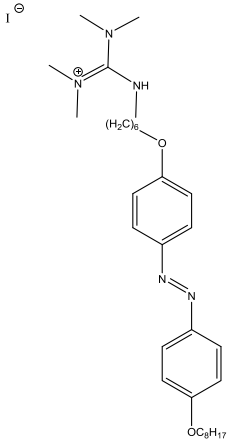
Analysis Info

Analysis Name	Laschat-Wuckert WUK 1062_9_01_22984.d	Acquisition Date	05.02.2014 08:24:04
Method	test-withloop.m		
Sample Name	Laschat-Wuckert WUK 1062	Operator	wo/tri
Comment		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





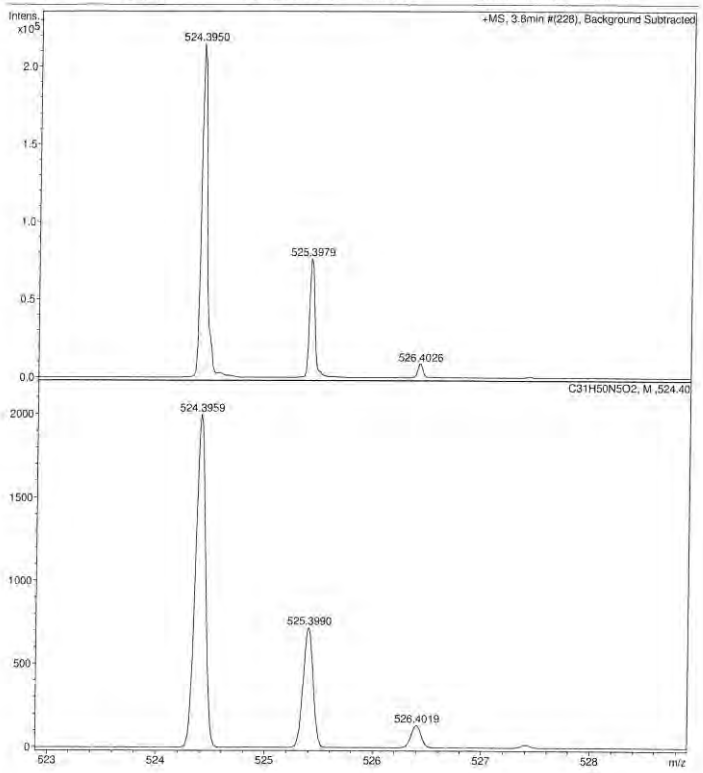
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	Laschat-Wuckert WUK 1062_9_01_22984.d	Acquisition Date	05.02.2014 08:24:04
Method	test-withloop.m	Operator	wo/tri
Sample Name	Laschat-Wuckert WUK 1062	Instrument	micrOTOF-Q 43
Comment			

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



Wuckert

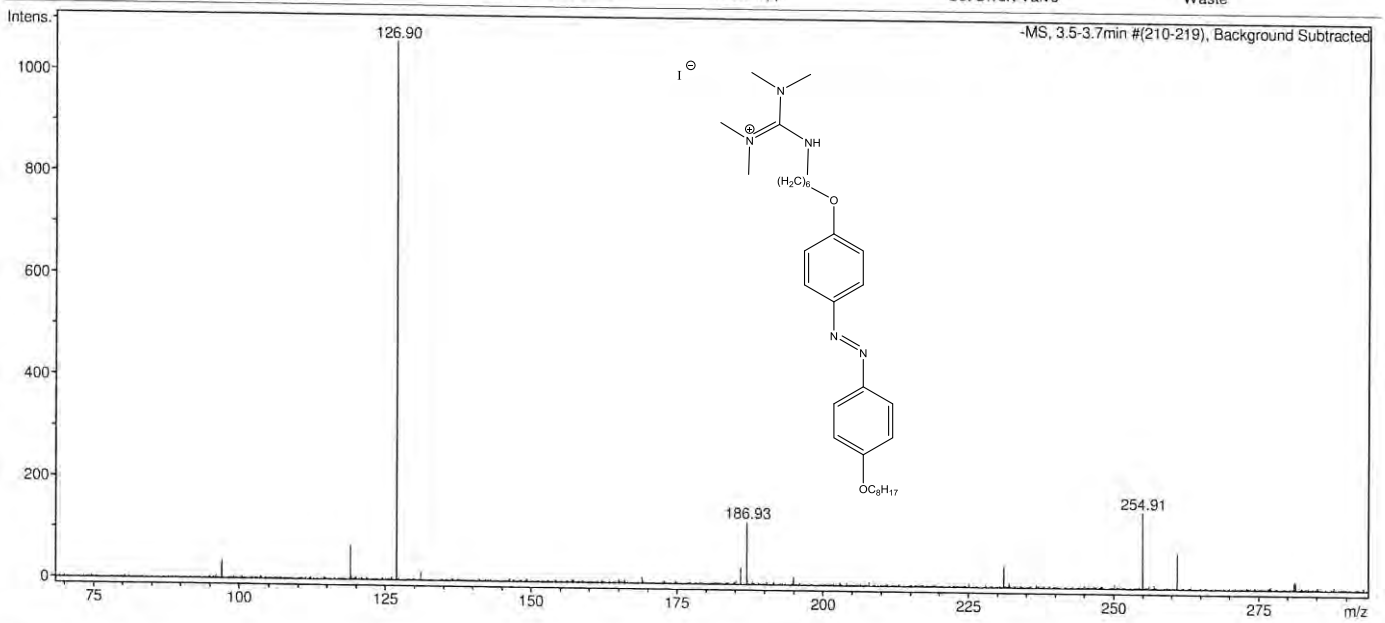
Massenspektrometrie - Universität Stuttgart

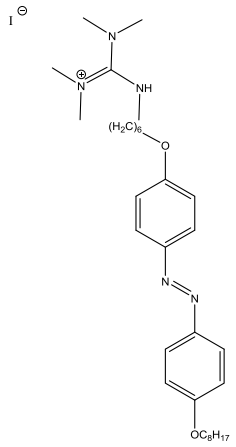
Analysis Info

Analysis Name	Laschat-Wuckert WUK 1062_9_01_22989.d	Acquisition Date	05.02.2014 08:55:11
Method	loop-tune-low-negativ.m		
Sample Name	Laschat-Wuckert WUK 1062	Operator	wo/tri
Comment		Instrument	micrOTOF-Q 43

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.8 Bar
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





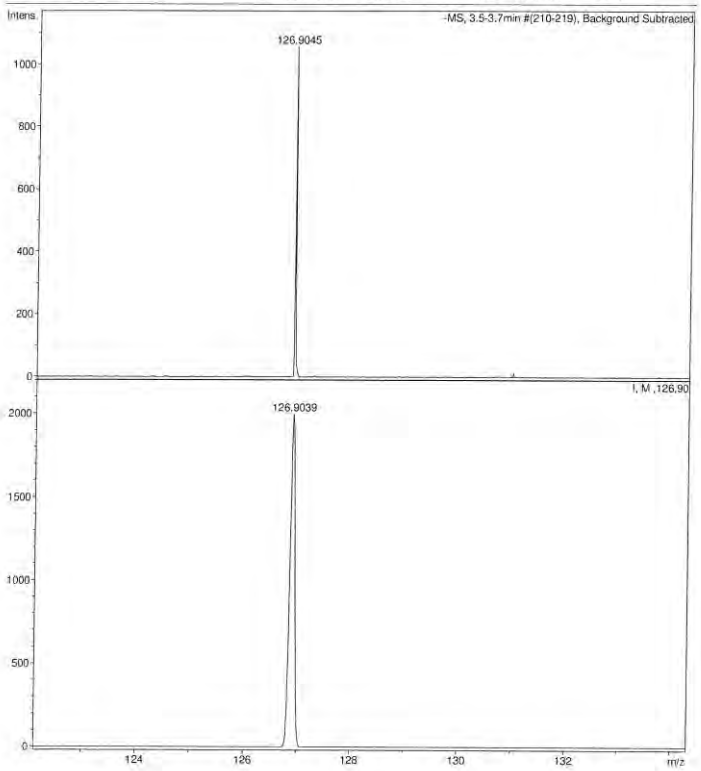
Massenspektrometrie - Universität Stuttgart

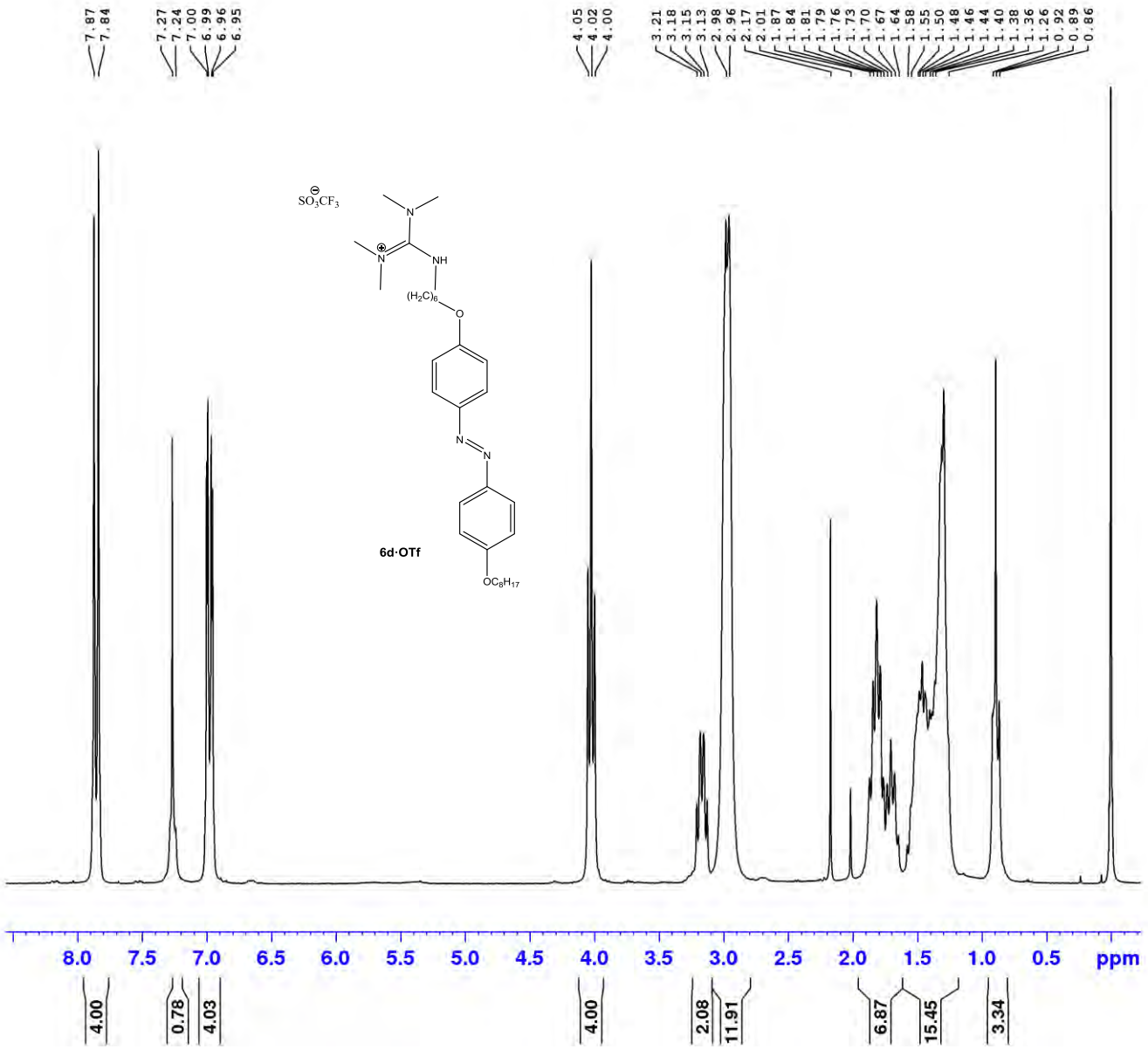
Analysis Info

Analysis Name	Laschat-Wuckert WUK 1062_9_01_22989.d	Acquisition Date	05.02.2014 08:55:11
Method	loop-tune-low-negativ.m	Operator	wo/tri
Sample Name	Laschat-Wuckert WUK 1062	Instrument	micrOTOF-Q 43
Comment			

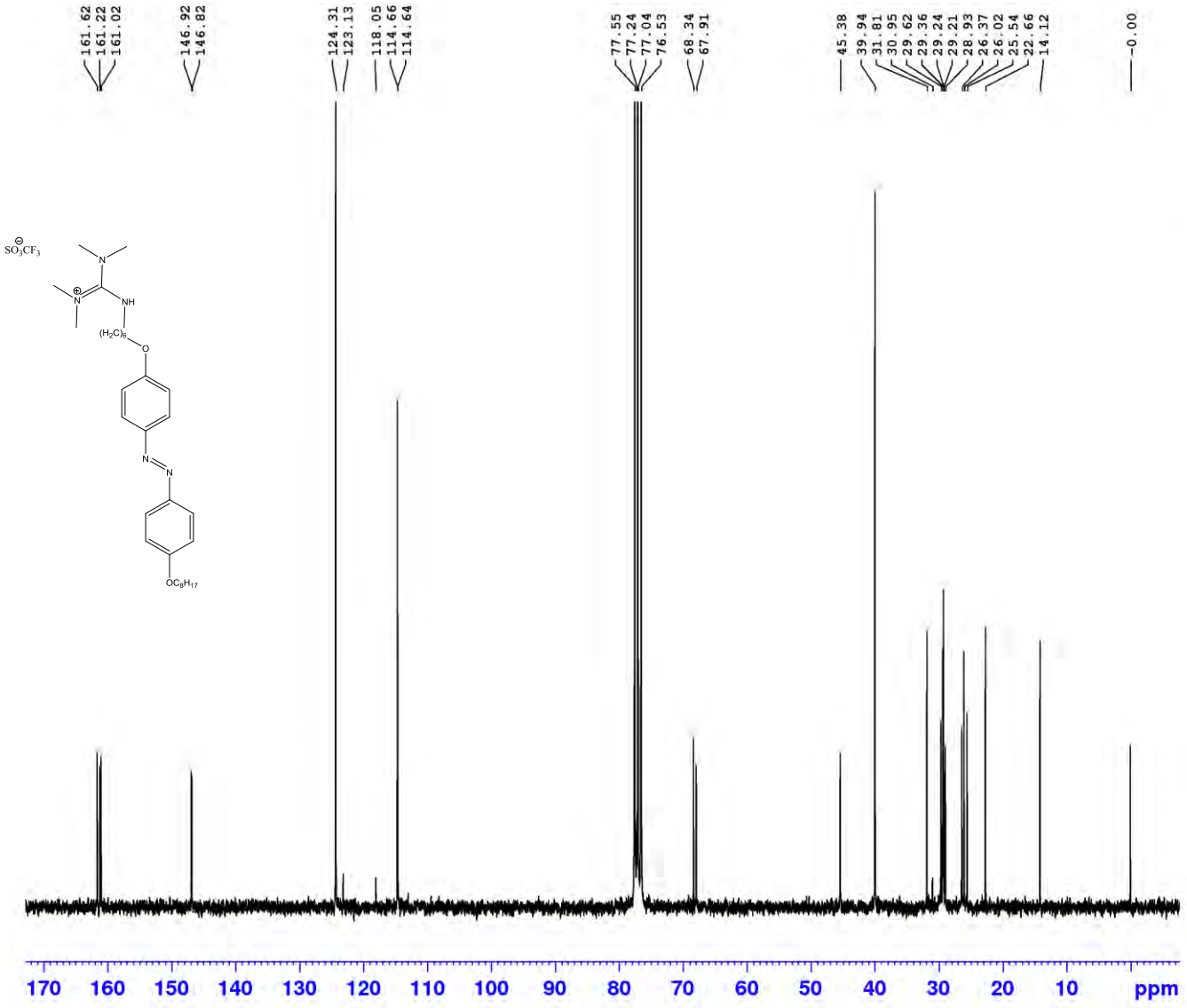
Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.8 Bar
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



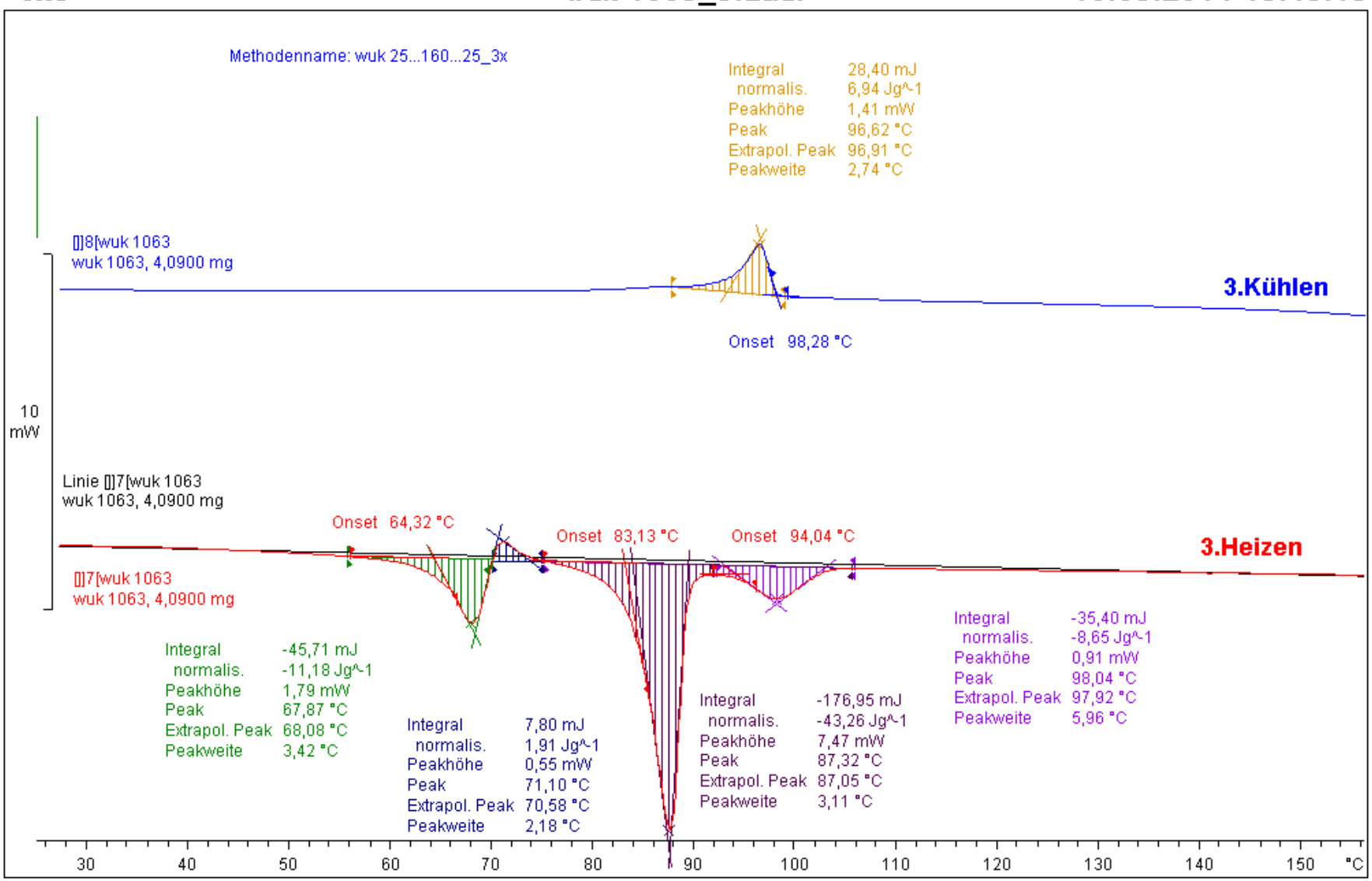


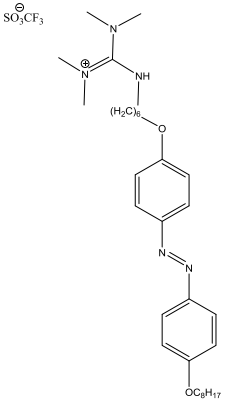

```
Current Data Parameters
NAME                  Jan31-2014
EXPNO                        400
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20140201
Time                        5.39
INSTRUM                    spect
PROBHD    5 mm QNP 1H/13
PULPROG                     zg30
TD                         65536
SOLVENT                    CDCl3
NS                            64
DS                             2
SWH                     5175.983 Hz
FIDRES                  0.078979 Hz
AQ                    6.3307776 sec
RG                         228.1
DW                        96.600 usec
DE                         8.00 usec
TE                         300.0 K
D1                    1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                        10.40 usec
PL1                       -6.00 dB
SFO1                250.1315447 MHz

F2 - Processing parameters
SI                         65536
SF                  250.1300060 MHz
WDW                           EM
SSB                0
LB                        0.30 Hz
GB                 0
PC                        1.00
```



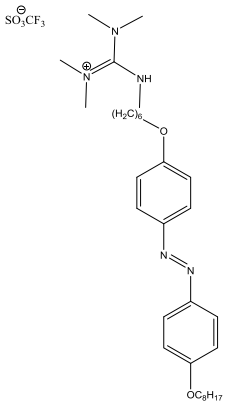

```
Current Data Parameters
NAME                  Jan31-2014
EXPNO                        401
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20140201
Time                        9.17
INSTRUM                    spect
PROBHD   5 mm QNP 1H/13
PULPROG                  zgpg30
TD                          65536
SOLVENT                   CDCl3
NS                           3072
DS                              4
SWH                  15060.241 Hz
FIDRES                0.229801 Hz
AQ                    2.1757953 sec
RG                       2896.3
DW                        33.200 usec
DE                         8.00 usec
TE                        300.0 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         13C
P1                         11.70 usec
PL1        0 dB
SFO1                62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                         1H
PCPD2                    100.00 usec
PL2                       -6.00 dB
PL12                      18.50 dB
PL13                      15.00 dB
SFO2                250.1310005 MHz

F2 - Processing parameters
SI                           32768
SF                   62.8952402 MHz
WDW                             EM
SSB        0
LB                         1.00 Hz
GB         0
PC                         1.40
```

^exo wuk 1063_3.Lauf 18.09.2014 15:49:19

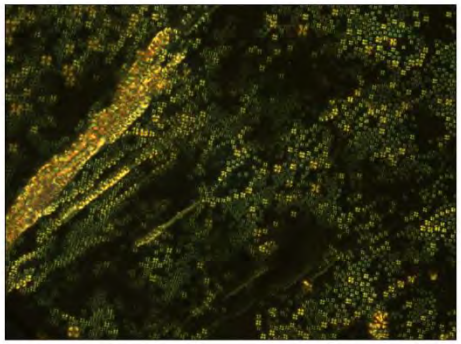




Uni Stuttgart - AK Laschat: Wuckert METTLER TOLEDO STAR^{e} SW 7.01

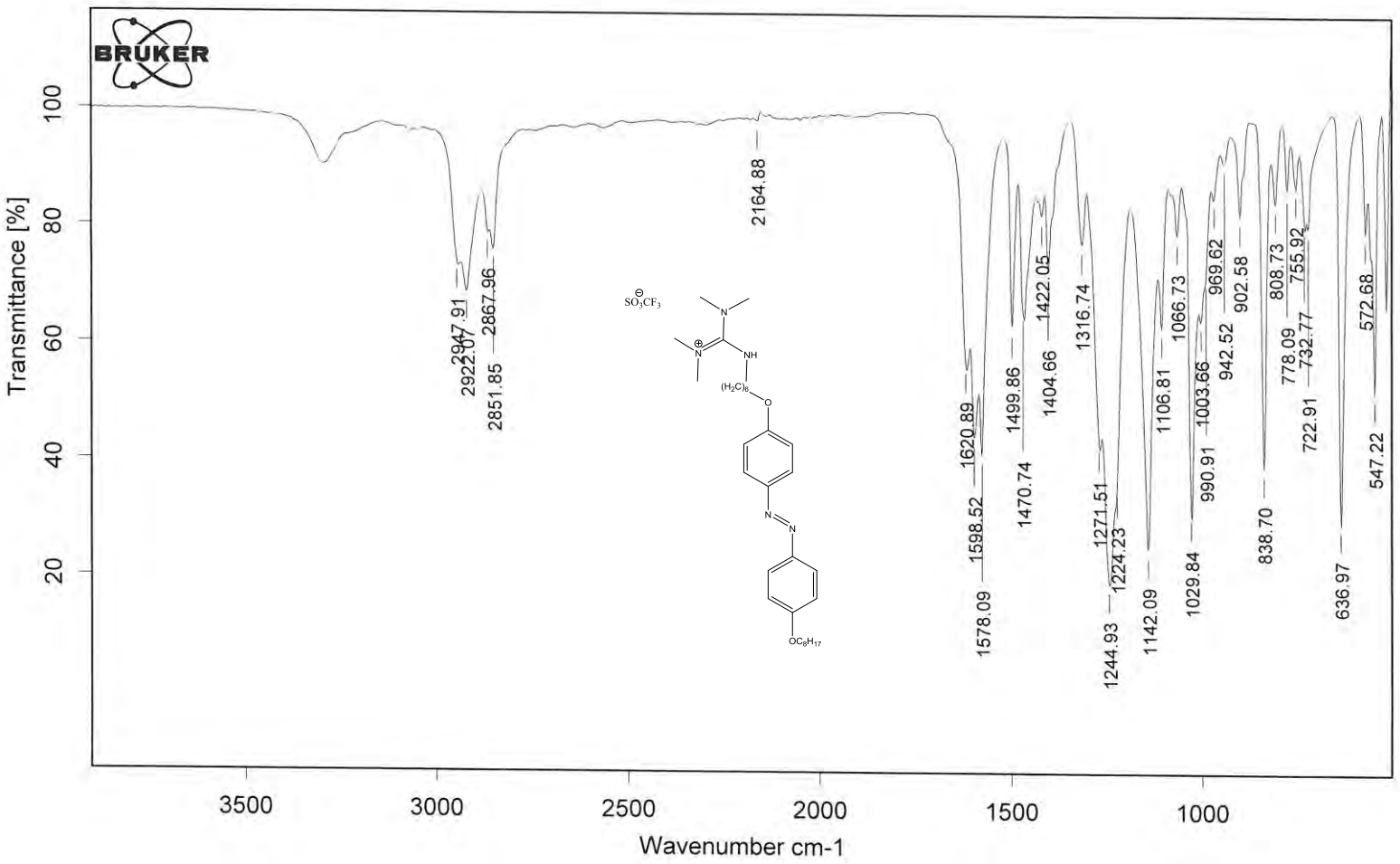


8 Sp 6 Triflat (wuk 1063)



Bildname: wuk 1063.2.2
Bildkommentar: Heizen mit 10°/min
bei 95° einige min. gestanden
100x

Bildname: wuk 1063.5
Bildkommentar: Kühlen von I ca. 100° mit 1°/min , länger bei 96°
dann mit 5°/min
aufgen. bei 82° - Phasenänder. - graue kleine Text.
200x



D:\IR-DATEN\twiehaus\1063.0	Wuckert/1063	fest	31/01/2014

Uncert

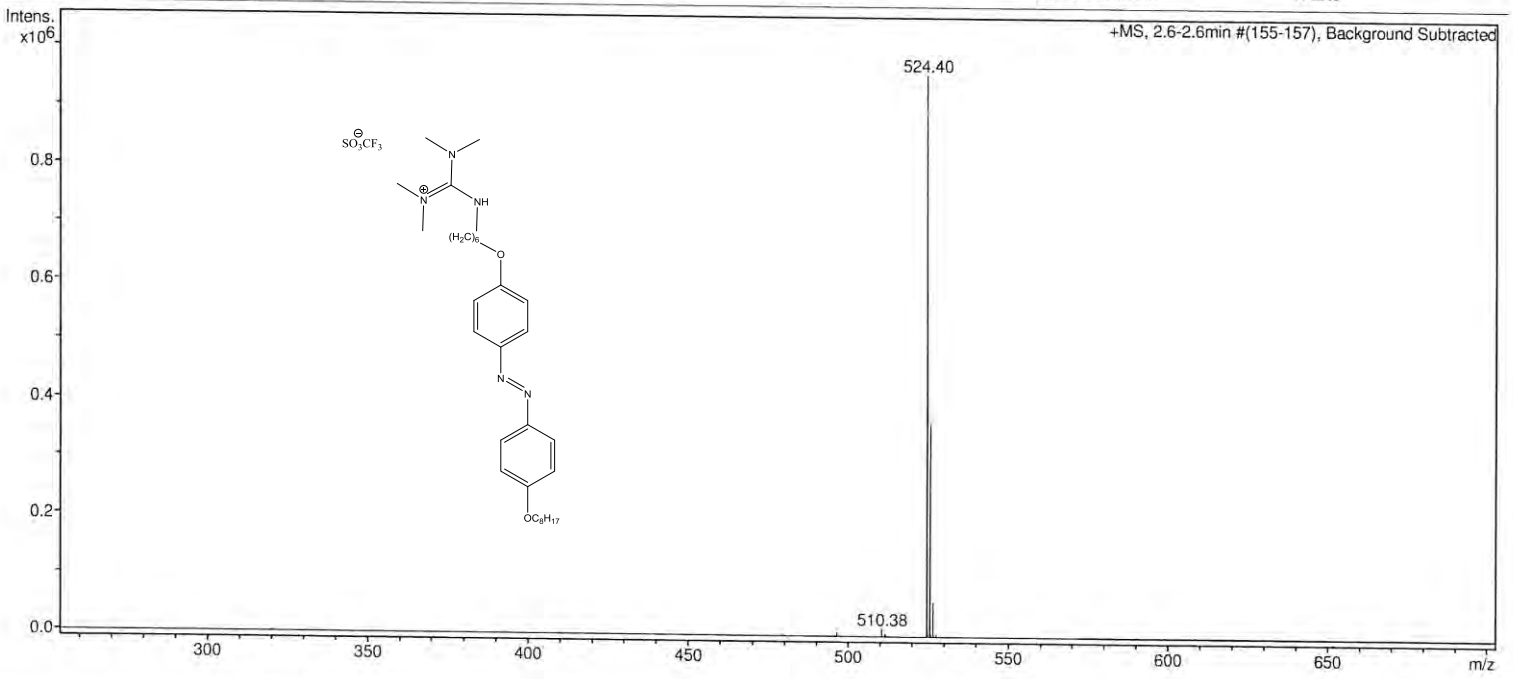
Massenspektrometrie - Universität Stuttgart

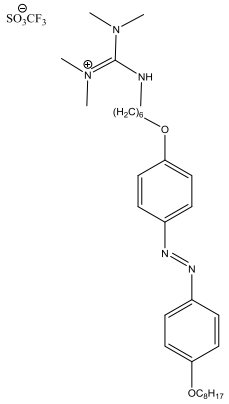
Analysis Info

Analysis Name	Laschat-Wuckert WUK 1063_10_01_22985.d	Acquisition Date	05.02.2014 08:30:26
Method	test-withloop.m		
Sample Name	Laschat-Wuckert WUK 1063	Operator	wo/tri
Comment		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





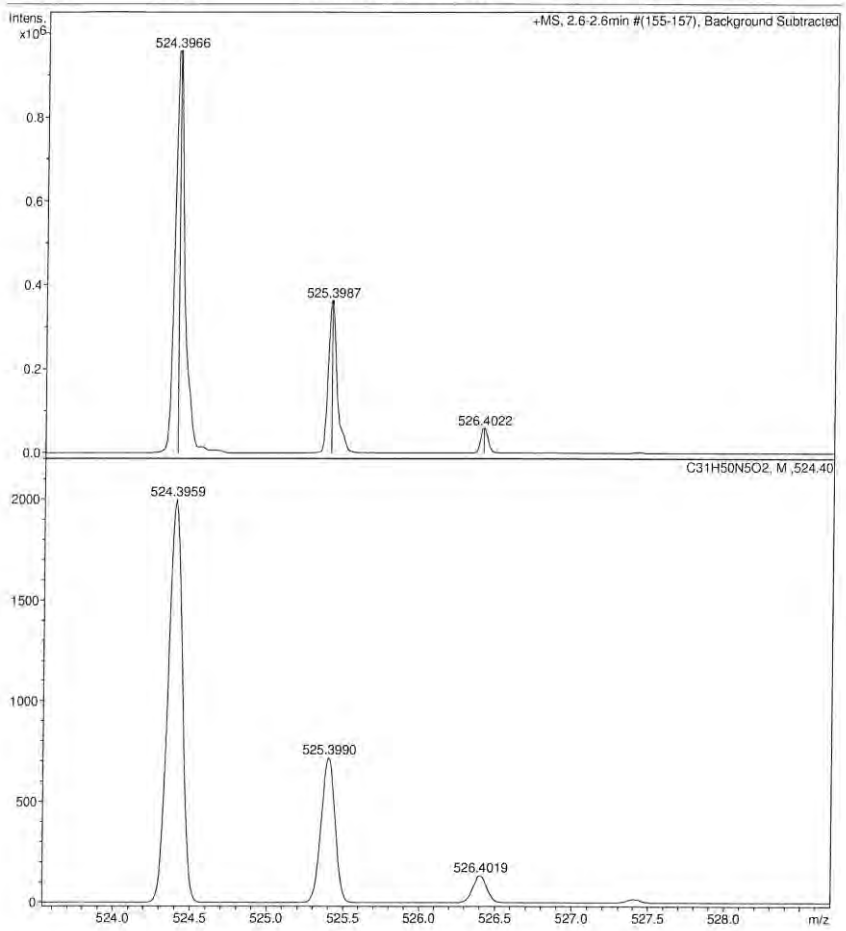
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	Laschat-Wuckert WUK 1063_10_01_22985.d	Acquisition Date	05.02.2014 08:30:26
Method	test-withloop.m	Operator	wo/tri
Sample Name	Laschat-Wuckert WUK 1063	Instrument	micrOTOF-Q 43
Comment			

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



Wuckert

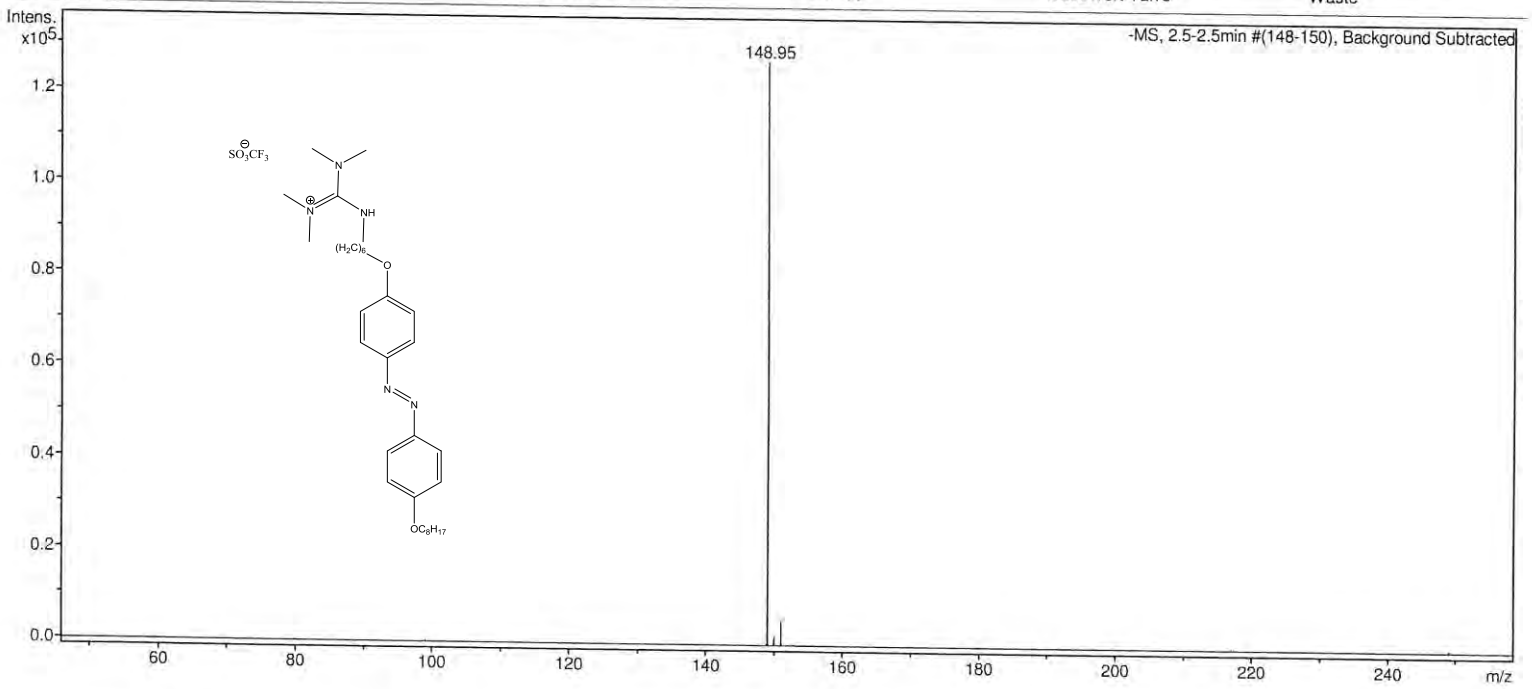
Massenspektrometrie - Universität Stuttgart

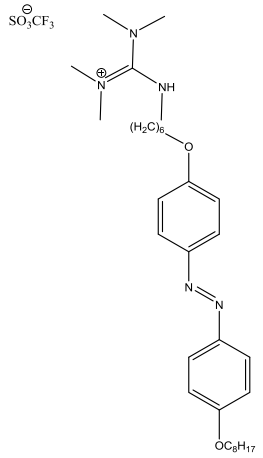
Analysis Info

Analysis Name	Laschat-Wuckert WUK 1063_10_01_22990.d	Acquisition Date	05.02.2014 09:01:26
Method	loop-tune-low-negativ.m		
Sample Name	Laschat-Wuckert WUK 1063	Operator	wo/tri
Comment		Instrument	micrOTOF-Q 43

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.8 Bar
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





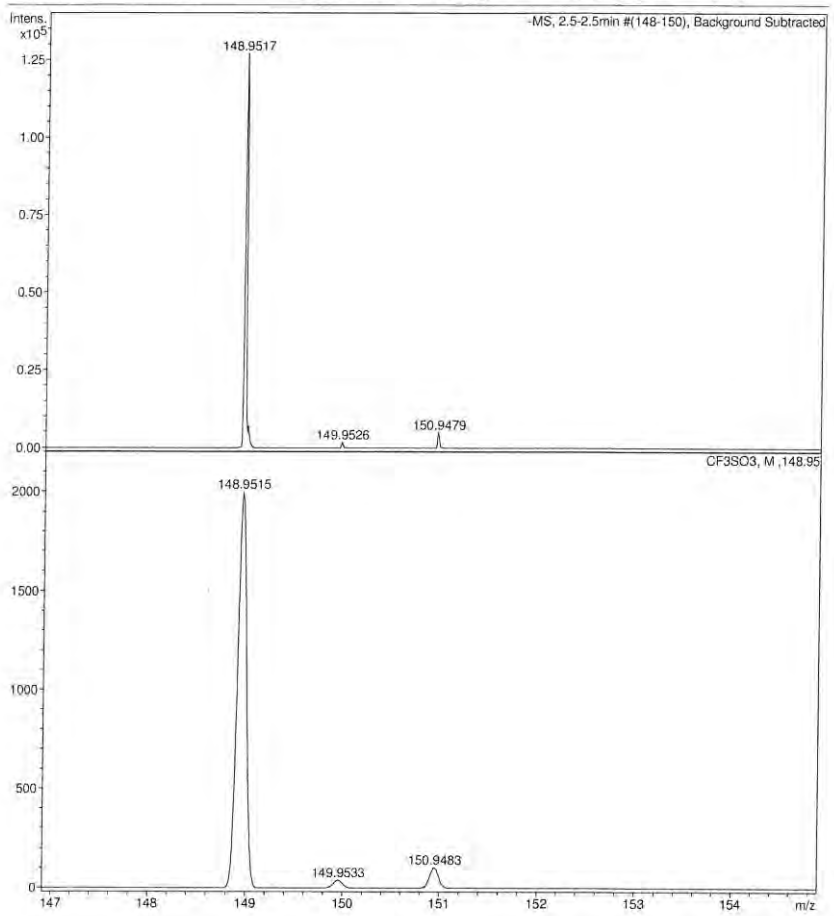
Massenspektrometrie - Universität Stuttgart

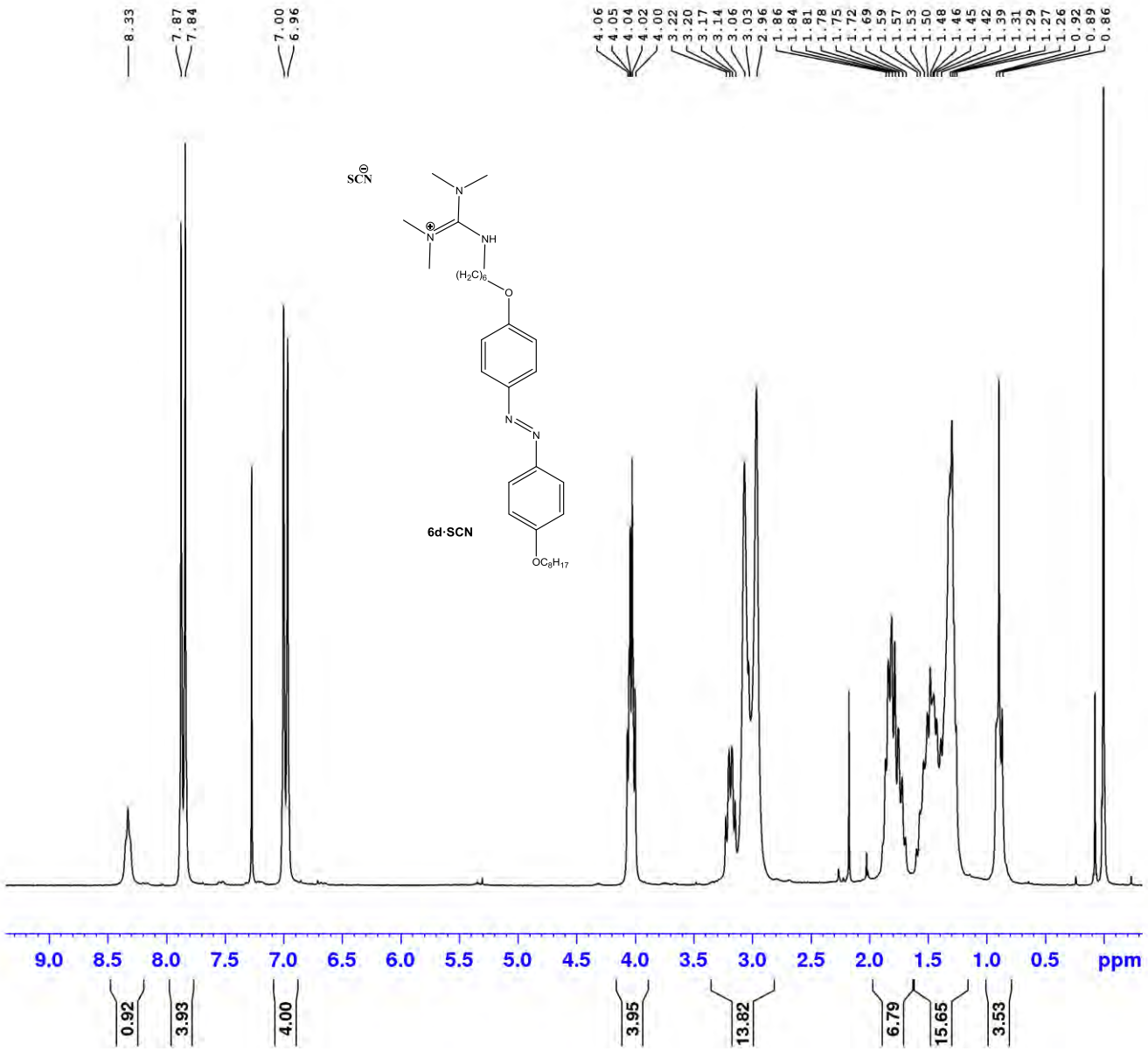
Analysis Info

Analysis Name	Laschat-Wuckert WUK 1063_10_01_22990.d	Acquisition Date	05.02.2014 09:01:26
Method	loop-tune-low-negativ.m	Operator	wo/tri
Sample Name	Laschat-Wuckert WUK 1063	Instrument	micrOTOF-Q 43
Comment			

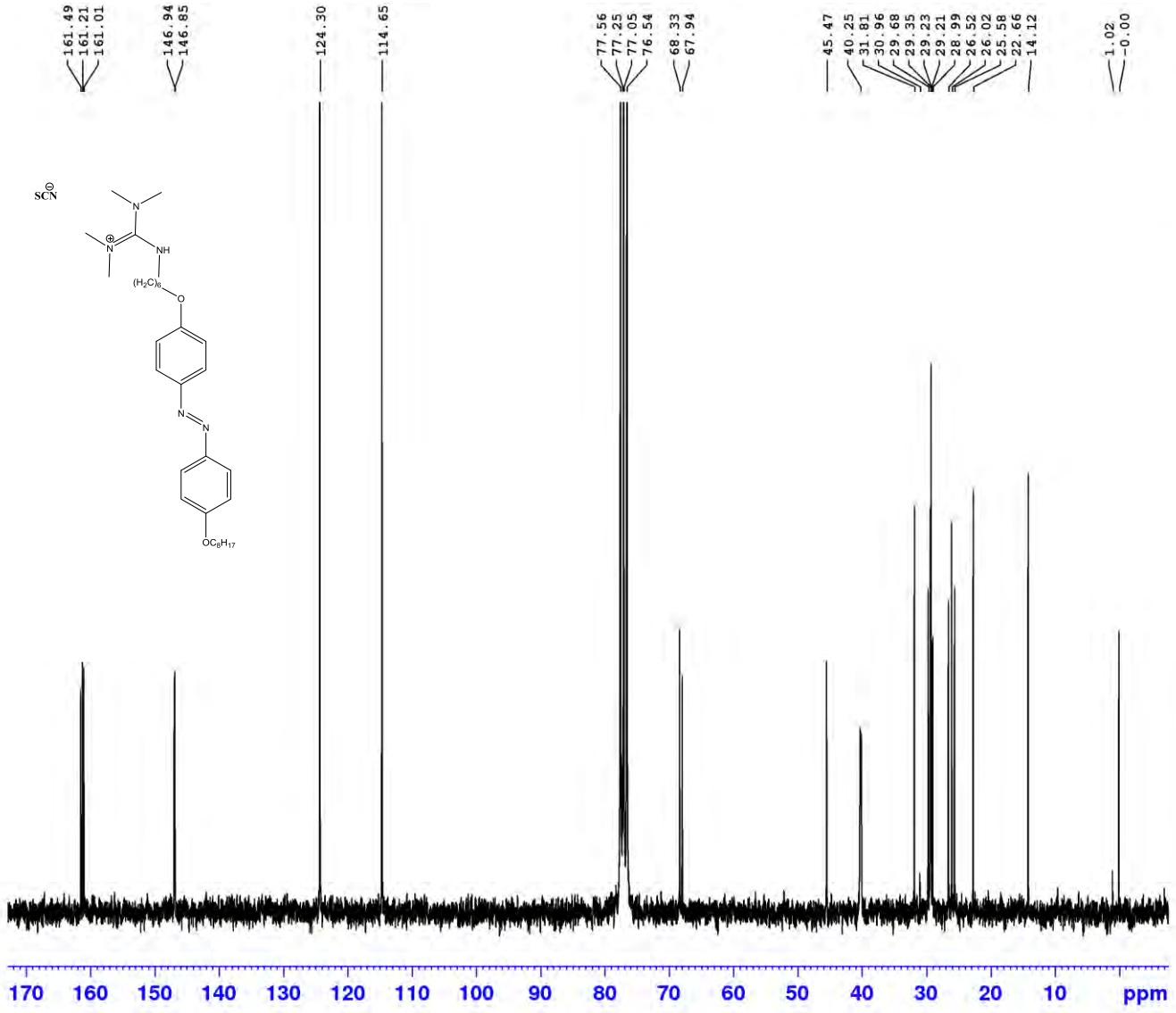
Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.8 Bar
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



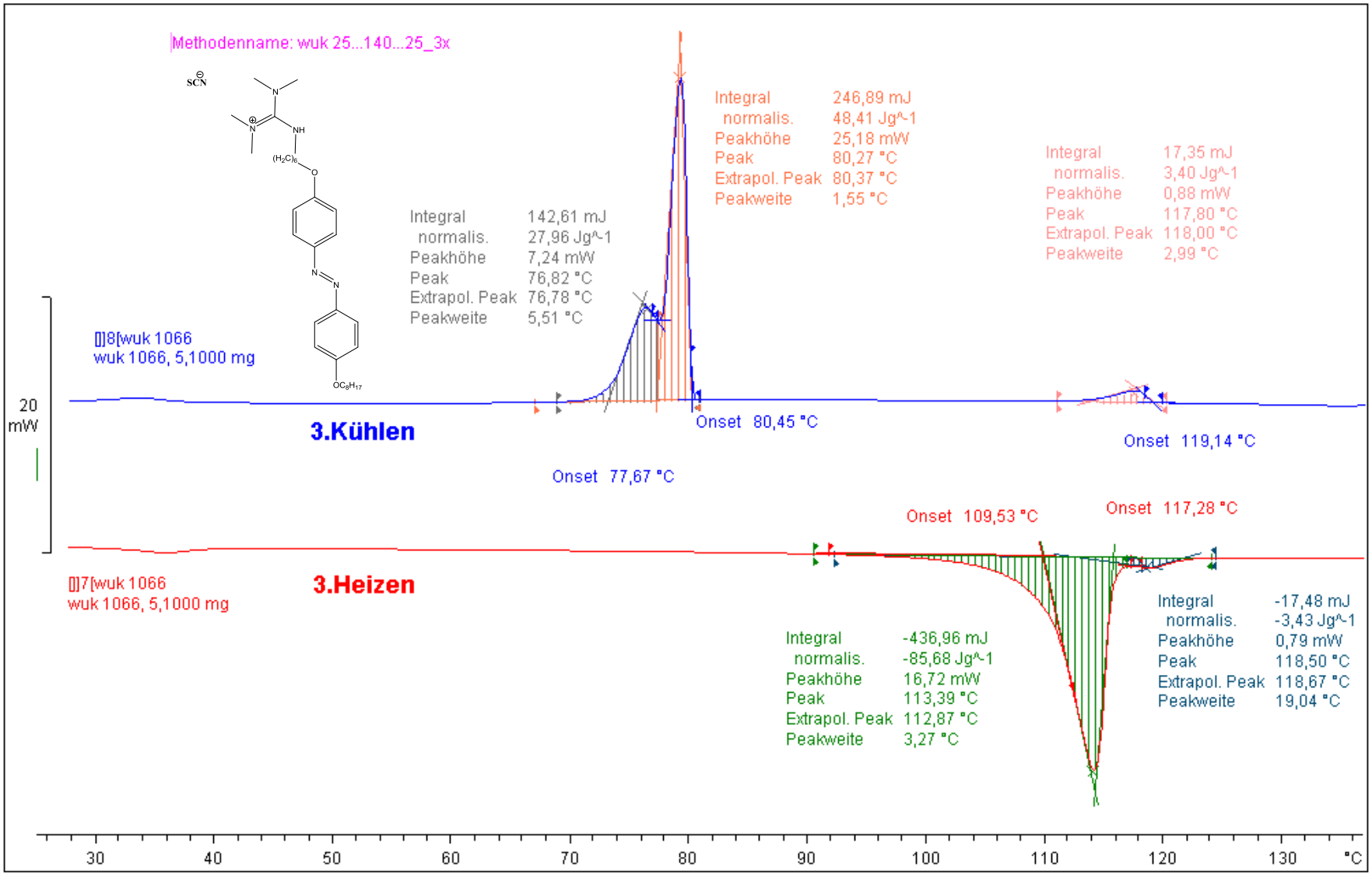



```
Current Data Parameters
NAME                  Jan31-2014
EXPNO                        380
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20140131
Time                       21.56
INSTRUM                    spect
PROBHD    5 mm QNP 1H/13
PULPROG                     zg30
TD                         65536
SOLVENT                    CDCl3
NS                            64
DS                             2
SWH                    5175.983 Hz
FIDRES                 0.078979 Hz
AQ                     6.3307776 sec
RG                         228.1
DW                        96.600 usec
DE                         8.00 usec
TE                         300.0 K
D1                     1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                        10.40 usec
PL1                       -6.00 dB
SFO1                250.1315447 MHz

F2 - Processing parameters
SI                         65536
SF                  250.1300051 MHz
WDW                           EM
SSB                0
LB                         0.30 Hz
GB                 0
PC                         1.00
```

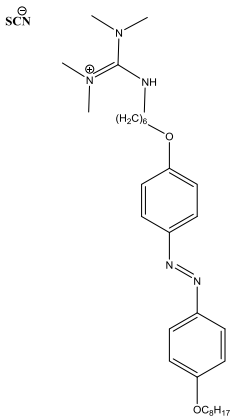



```
Current Data Parameters
NAME                  Jan31-2014
EXPNO                        381
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20140201
Time                        1.34
INSTRUM                    spect
PROBHD   5 mm QNP 1H/13
PULPROG                  zgpg30
TD                          65536
SOLVENT                     CDC13
NS                           3072
DS                              4
SWH                  15060.241 Hz
FIDRES                0.229801 Hz
AQ                   2.1757953 sec
RG                      2896.3
DW                      33.200 usec
DE                       8.00 usec
TE                       300.0 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                         13C
P1                         11.70 usec
PL1       0 dB
SFO1                62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                         1H
PCPD2                    100.00 usec
PL2                       -6.00 dB
PL12                      18.50 dB
PL13                      15.00 dB
SFO2                250.1310005 MHz

F2 - Processing parameters
SI                           32768
SF                  62.8952400 MHz
WDW                             EM
SSB       0
LB                        1.00 Hz
GB        0
PC                        1.40
```

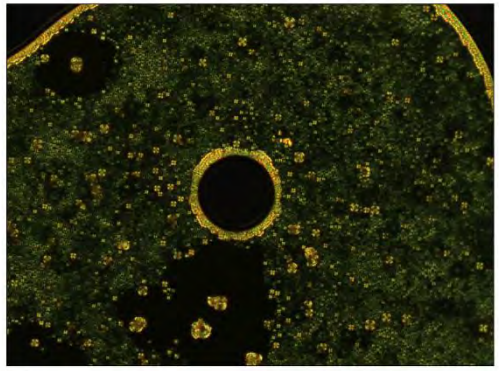
^exo wuk 1066_3.Lauf 18.09.2014 15:52:12



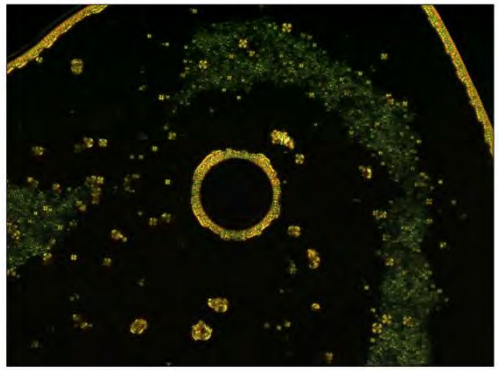
Uni Stuttgart - AK Laschat: Wuckert METTLER TOLEDO STAR^{e} SW 7.01



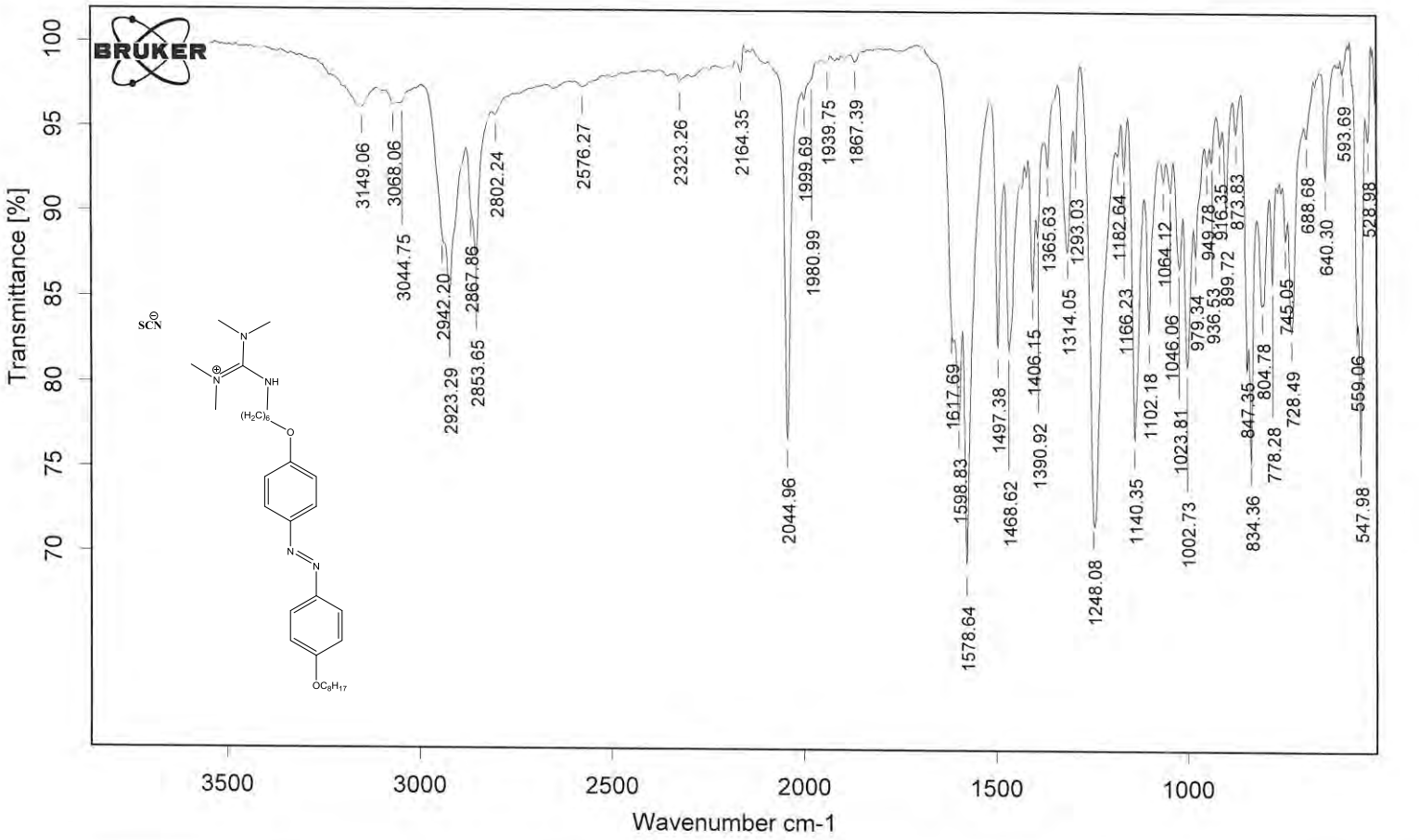
8 Sp 6 Thiocyanat (wuk 1066)



Bildname: wuk 1066.2
Bildkommentar: Kühlen von 122° I mit 1°/min
bei 121° die ersten Text.
aufgen. bei 117°
200x



Bildname: wuk 1066.3
Bildkommentar: Kühlen von 122° I mit 1°/min
bei 121° die ersten Text.
aufgen. bei 114.5°
200x



D:\IR-DATEN\twiehaus\1066.0	Wuckert/1066	fest	31/01/2014

Wuelrot

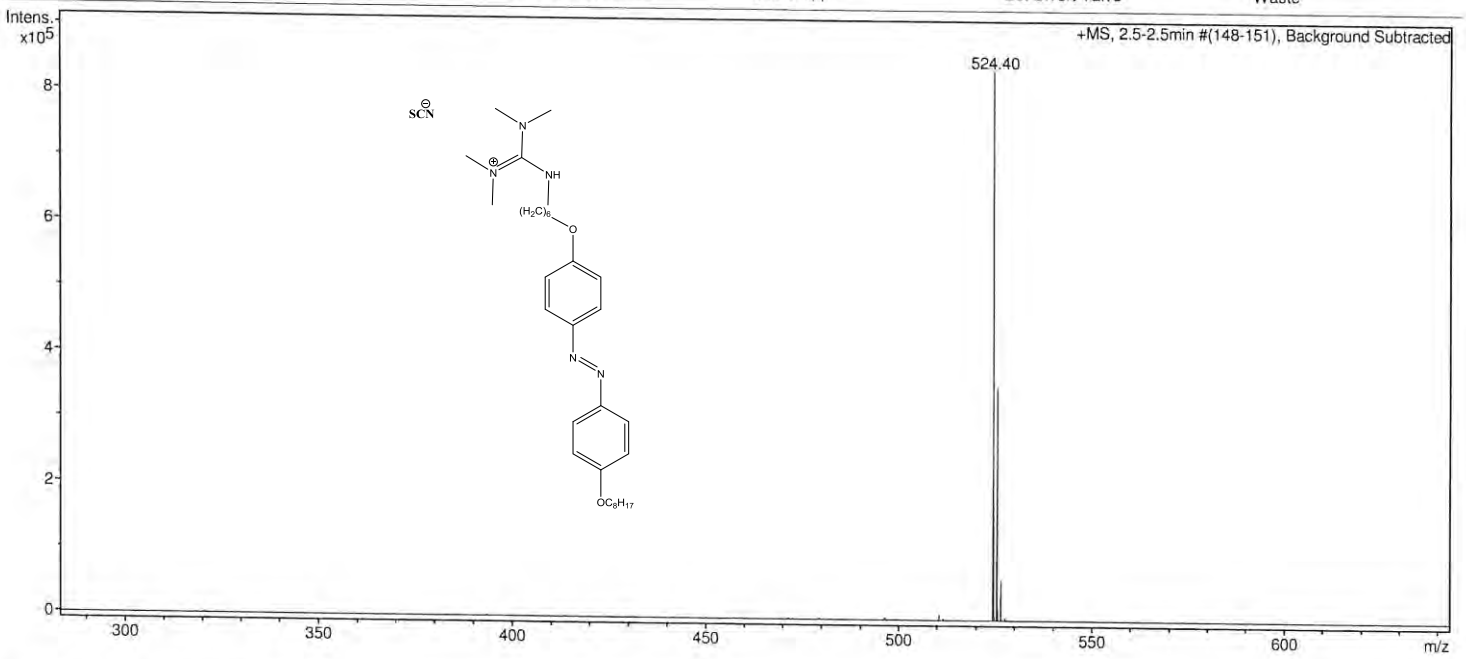
Massenspektrometrie - Universität Stuttgart

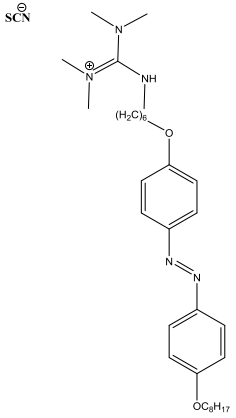
Analysis Info

Analysis Name	Laschat-Wuckert WUK 1066_13_01_22988.d	Acquisition Date	05.02.2014 08:48:42
Method	test-withloop.m		
Sample Name	Laschat-Wuckert WUK 1066	Operator	wo/tri
Comment		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





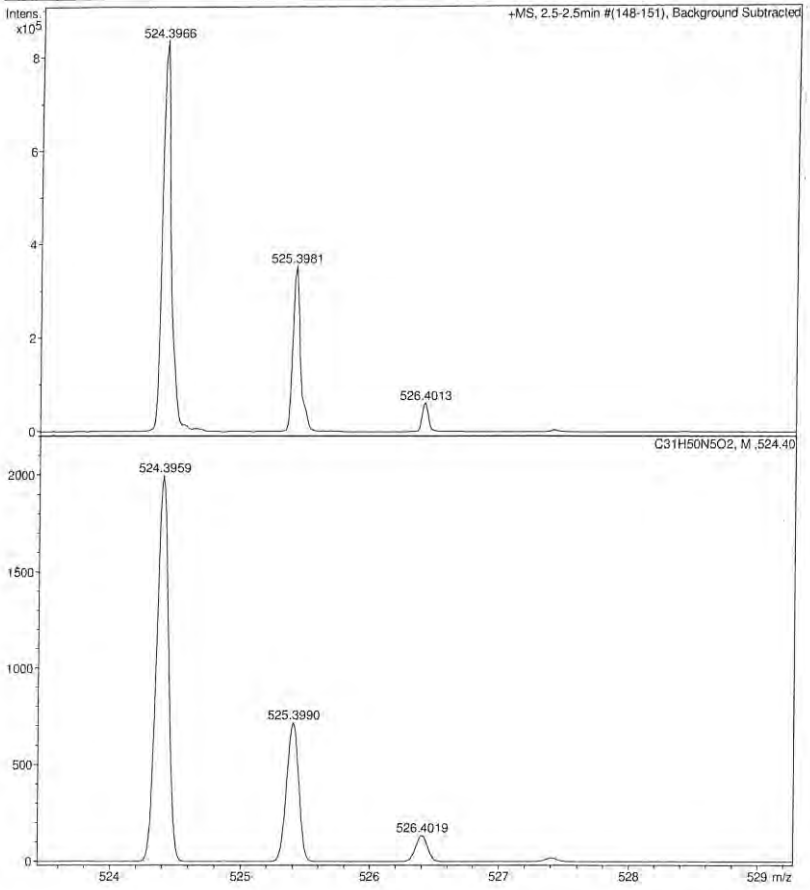
Massenspektrometrie - Universität Stuttgart

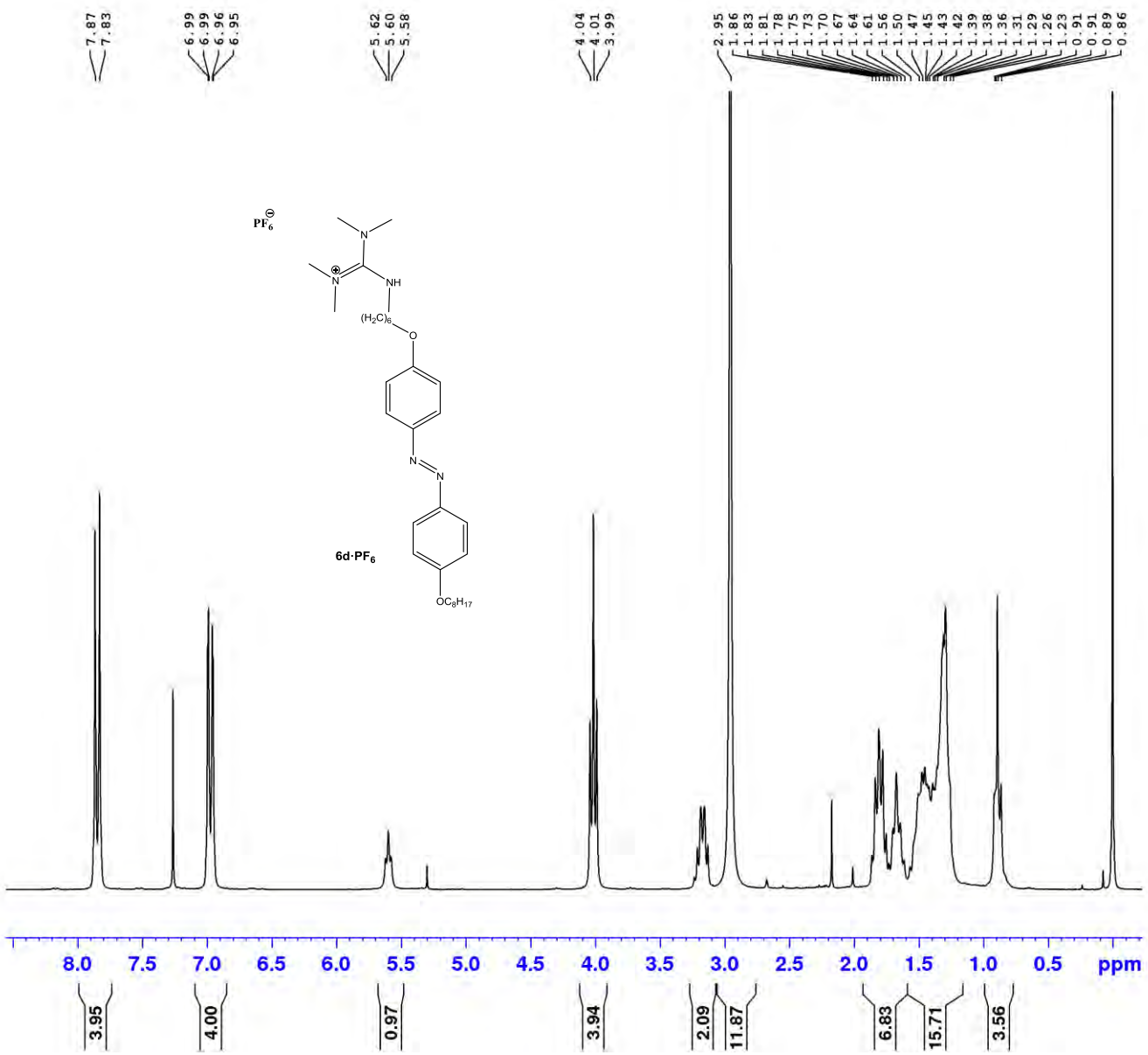
Analysis Info

Analysis Name	Laschat-Wuckert WUK 1066_13_01_22988.d	Acquisition Date	05.02.2014 08:48:42
Method	test-withloop.m	Operator	wo/tri
Sample Name	Laschat-Wuckert WUK 1066	Instrument	micrOTOF-Q 43
Comment			

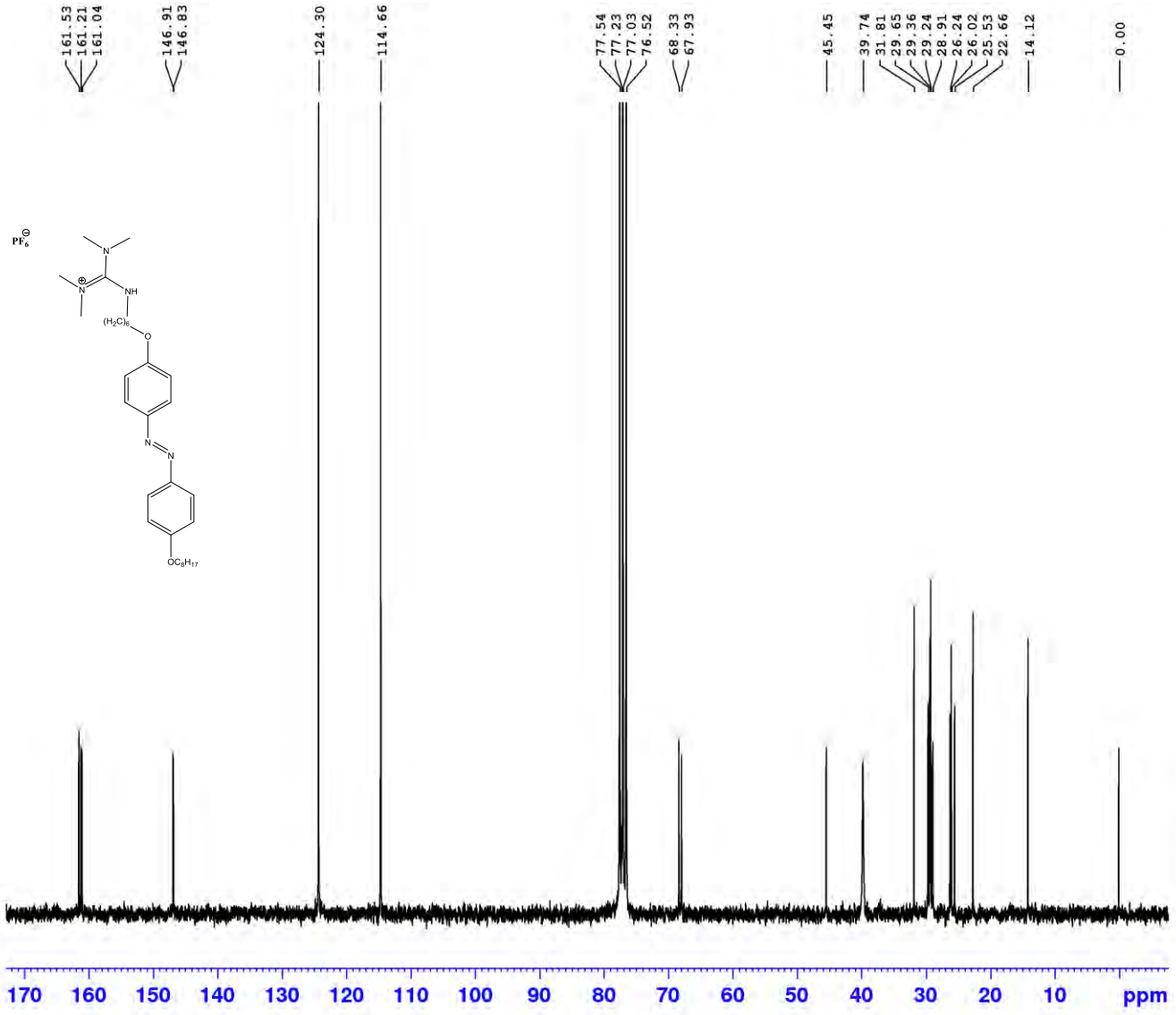
Acquisition Parameter

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



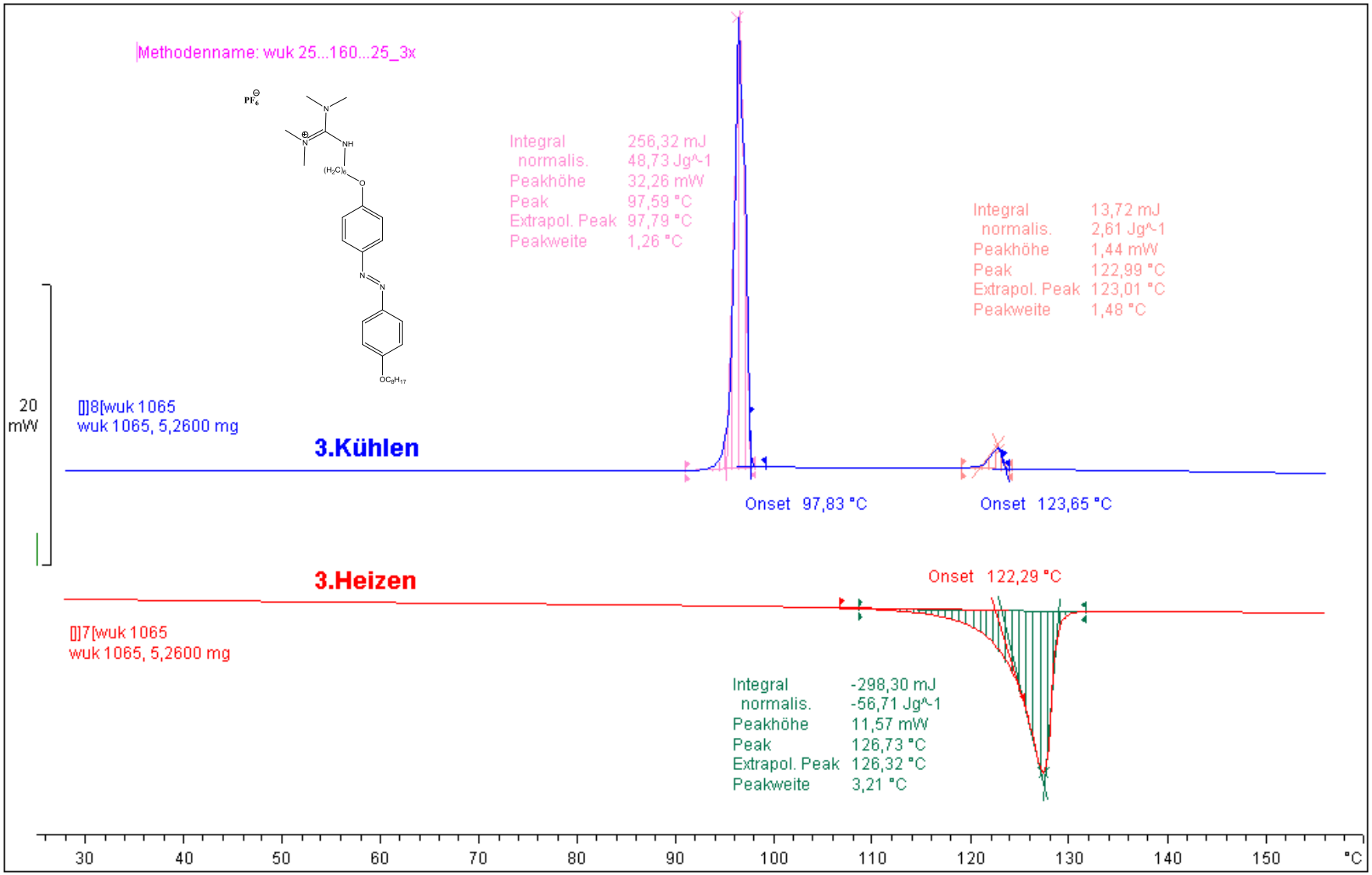



```
Current Data Parameters
NAME                  Jan31-2014
EXPNO                        420
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20140201
Time                       13.15
INSTRUM                    spect
PROBHD    5 mm QNP 1H/13
PULPROG                     zg30
TD                         65536
SOLVENT                    CDCl3
NS                            64
DS                             2
SWH                     5175.983 Hz
FIDRES                  0.078979 Hz
AQ                    6.3307776 sec
RG                         228.1
DW                        96.600 usec
DE                         8.00 usec
TE                         300.0 K
D1                    1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                         10.40 usec
PL1                        -6.00 dB
SFO1                  250.1315447 MHz

F2 - Processing parameters
SI                         65536
SF                    250.1300070 MHz
WDW                           EM
SSB                0
LB                         0.30 Hz
GB                 0
PC                         1.00
```



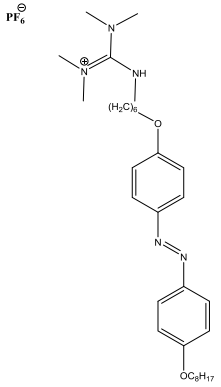

```
Current Data Parameters
NAME                  Jan31-2014
EXPNO                        421
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20140201
Time                       16.53
INSTRUM                    spect
PROBHD   5 mm QNP 1H/13
PULPROG                  zgpg30
TD                          65536
SOLVENT                     CDC13
NS                           3072
DS                              4
SWH                  15060.241 Hz
FIDRES                0.229801 Hz
AQ                    2.1757953 sec
RG                       2896.3
DW                        33.200 usec
DE                         8.00 usec
TE                        300.0 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                         13C
P1                         11.70 usec
PL1        0 dB
SFO1                62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                         1H
PCPD2                    100.00 usec
PL2                       -6.00 dB
PL12                      18.50 dB
PL13                      15.00 dB
SFO2                250.1310005 MHz

F2 - Processing parameters
SI                           32768
SF                   62.8952404 MHz
WDW                             EM
SSB        0
LB                         1.00 Hz
GB         0
PC                         1.40
```

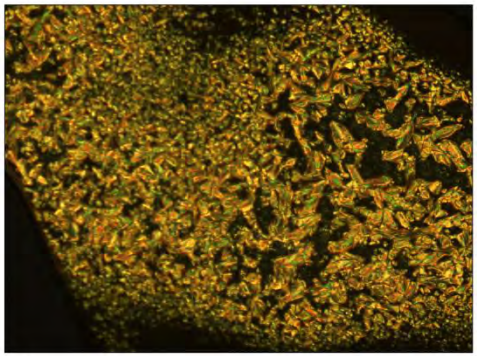
^exo wuk 1065_3.Lauf 18.09.2014 15:51:15



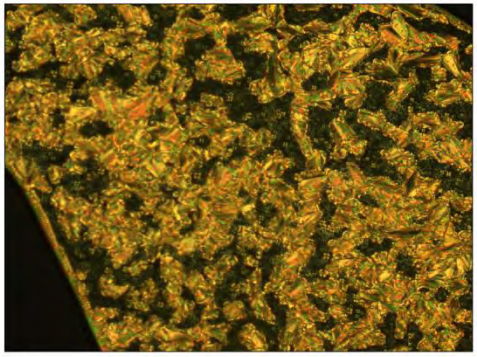
Uni Stuttgart - AK Laschat: Wuckert METTLER TOLEDO STARe SW 7.01

8 Sp 6 Hexafluorophosphat (wuk 1065)

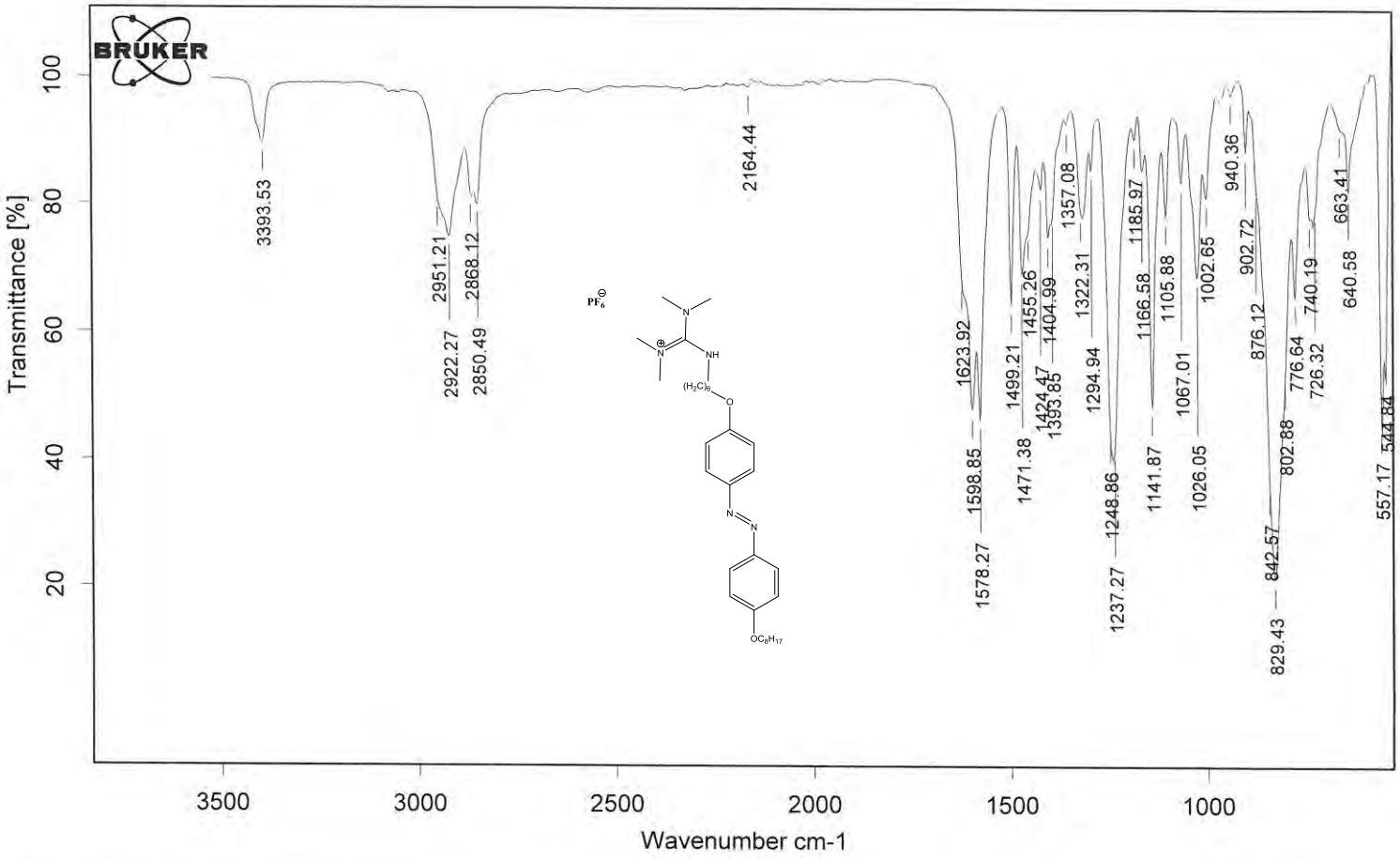




Bildname: wuk 1065.1
Bildkommentar: Kühlen von I (130°) mit 5°/min
bei 126.6° sehr schnell erschienen
100x



Bildname: wuk 1065.2
Bildkommentar: Kühlen von I (130°) mit 5°/min
bei 123°
100x



D:\IR-DATEN\twiehaus\1065.0	Wuckert/1065	fest	31/01/2014

Unclear

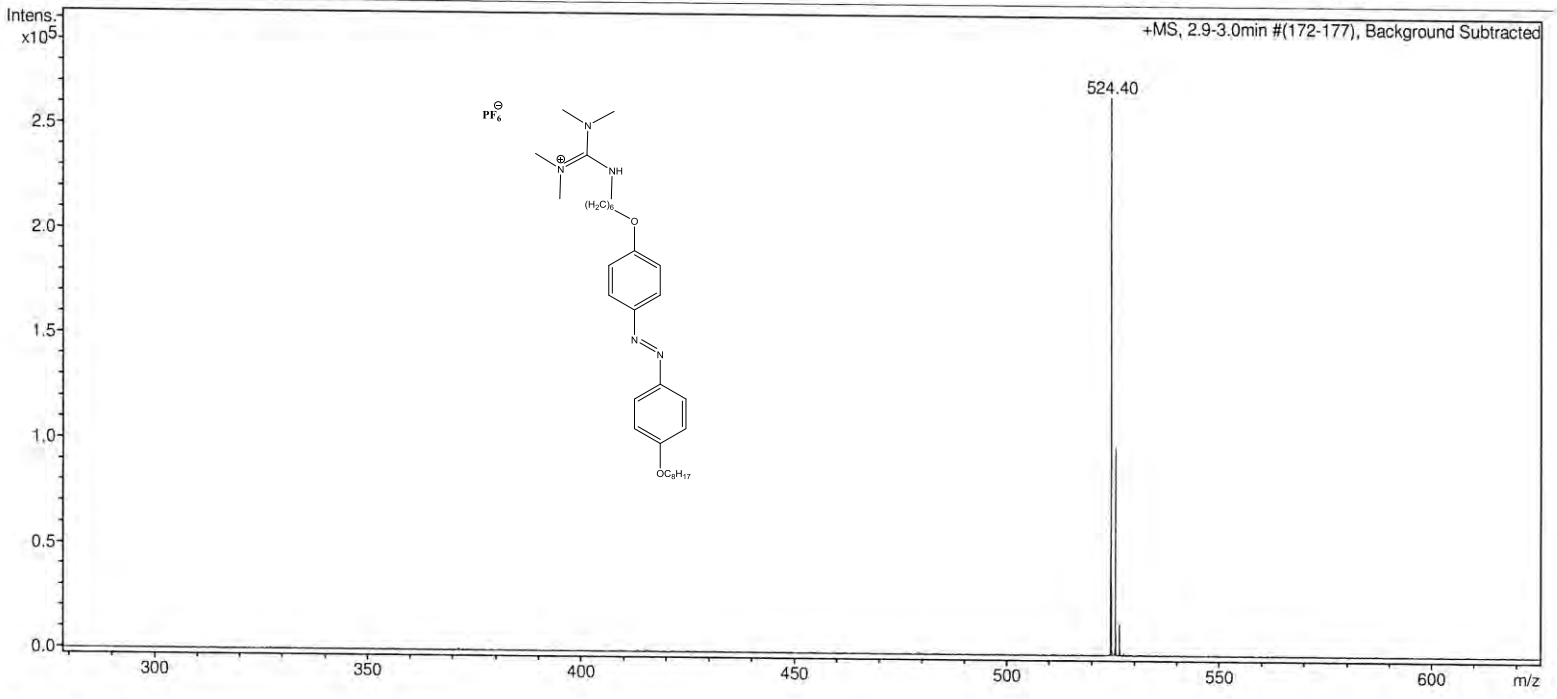
Massenspektrometrie - Universität Stuttgart

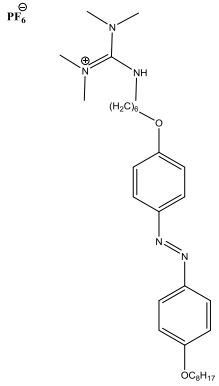
Analysis Info

Analysis Name	Laschat-Wuckert WUK 1065_12_01_22987.d	Acquisition Date	05.02.2014 08:42:37
Method	test-withloop.m	Operator	wo/tri
Sample Name	Laschat-Wuckert WUK 1065	Instrument	micrOTOF-Q 43
Comment			

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





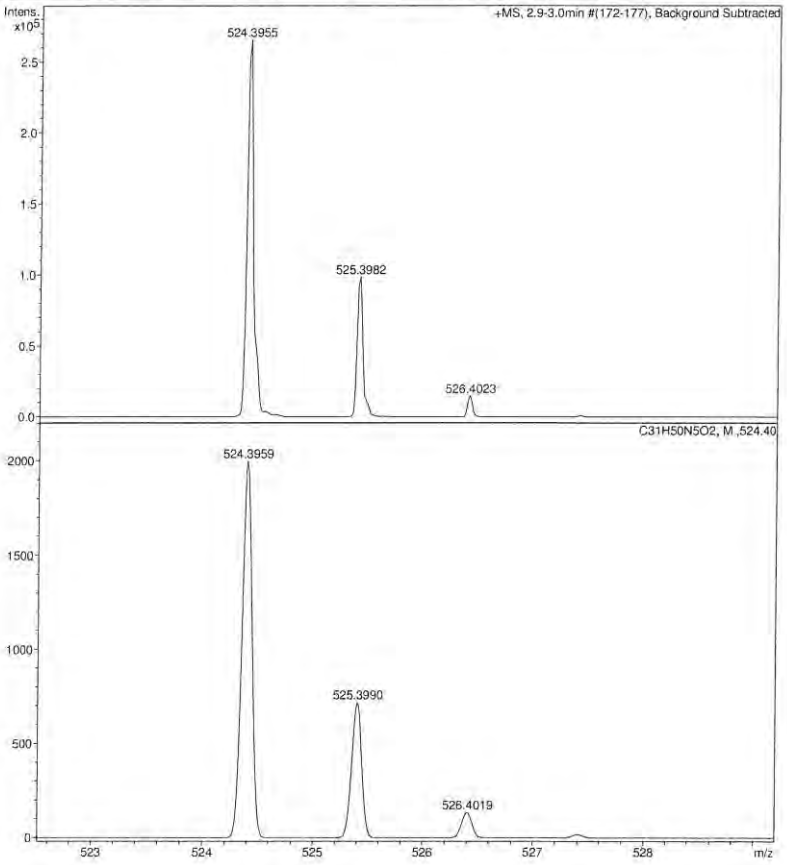
Massenspektrometrie - Universität Stuttgart

Analysis Info

Analysis Name	Laschat-Wuckert WUK 1065_12_01_22987.d	Acquisition Date	05.02.2014 08:42:37
Method	test-withloop.m	Operator	wo/tri
Sample Name	Laschat-Wuckert WUK 1065	Instrument	micrOTOF-Q 43
Comment			

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



Unkert

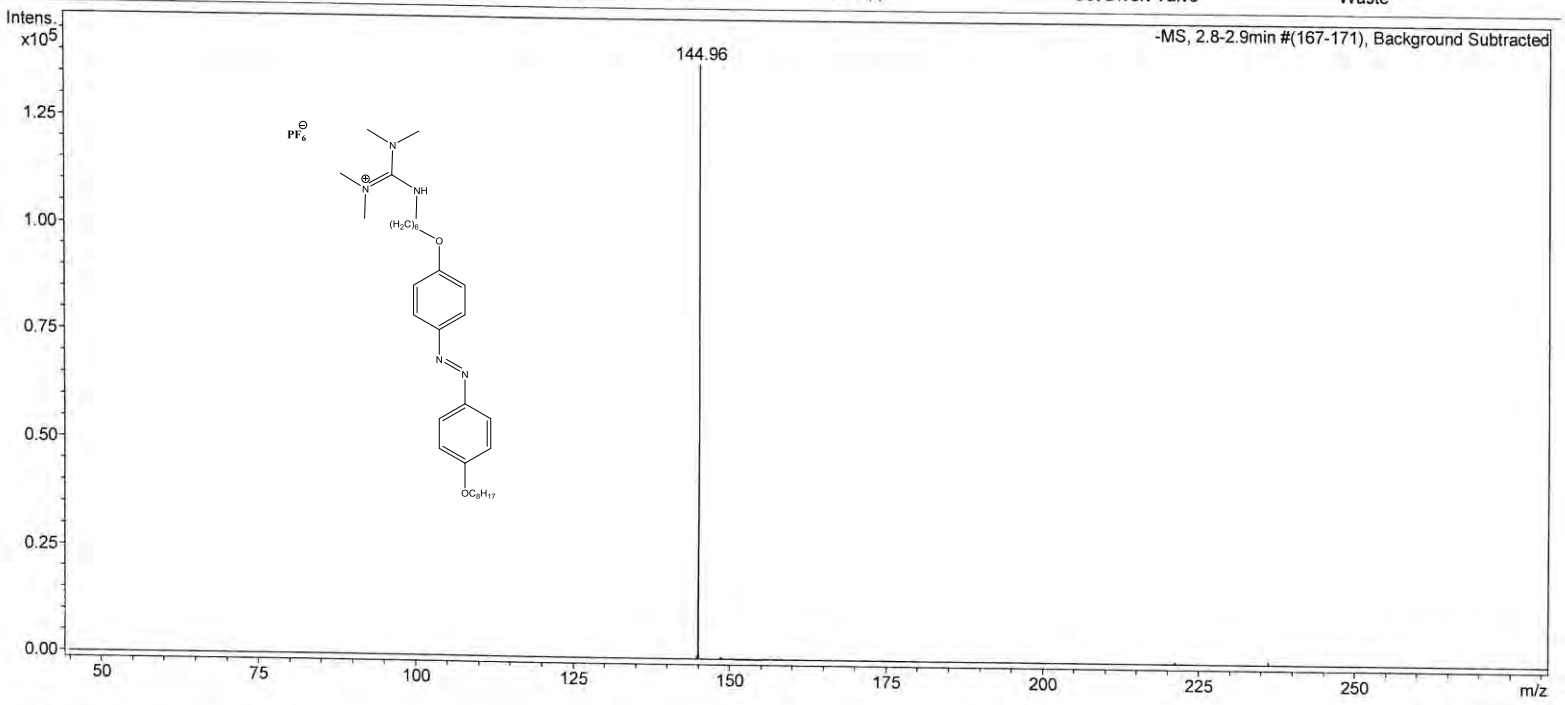
Massenspektrometrie - Universität Stuttgart

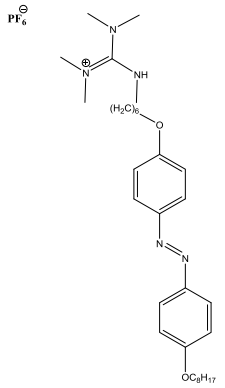
Analysis Info

Analysis Name	Laschat-Wuckert WUK 1065_12_01_22992.d	Acquisition Date	05.02.2014 09:13:41
Method	loop-tune-low-negativ.m		
Sample Name	Laschat-Wuckert WUK 1065	Operator	wo/tri
Comment		Instrument	micrOTOF-Q 43

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.8 Bar
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





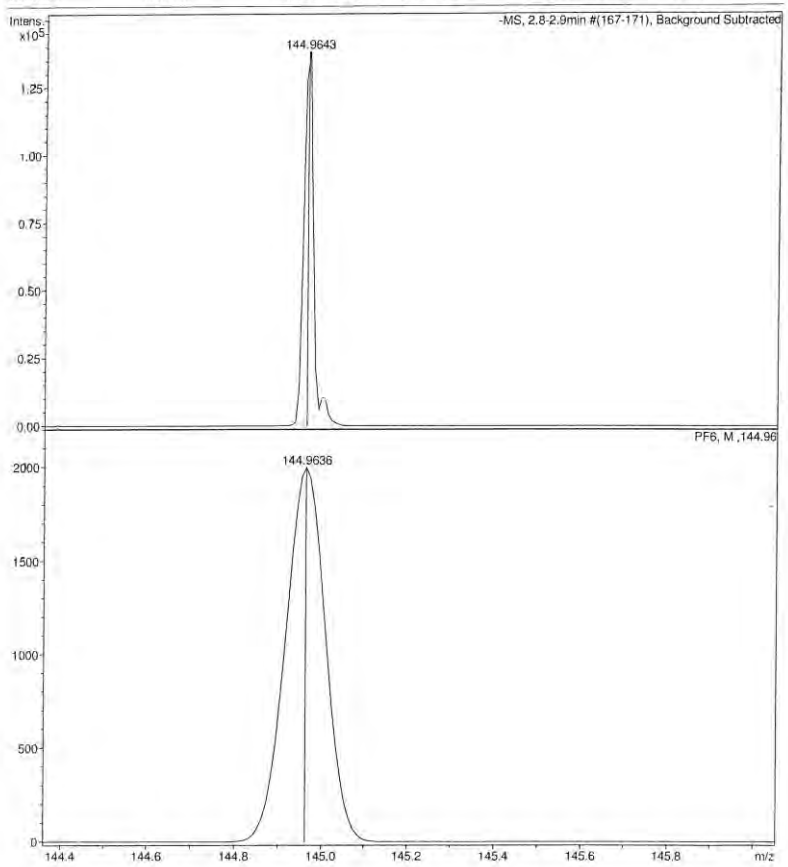
Massenspektrometrie - Universität Stuttgart

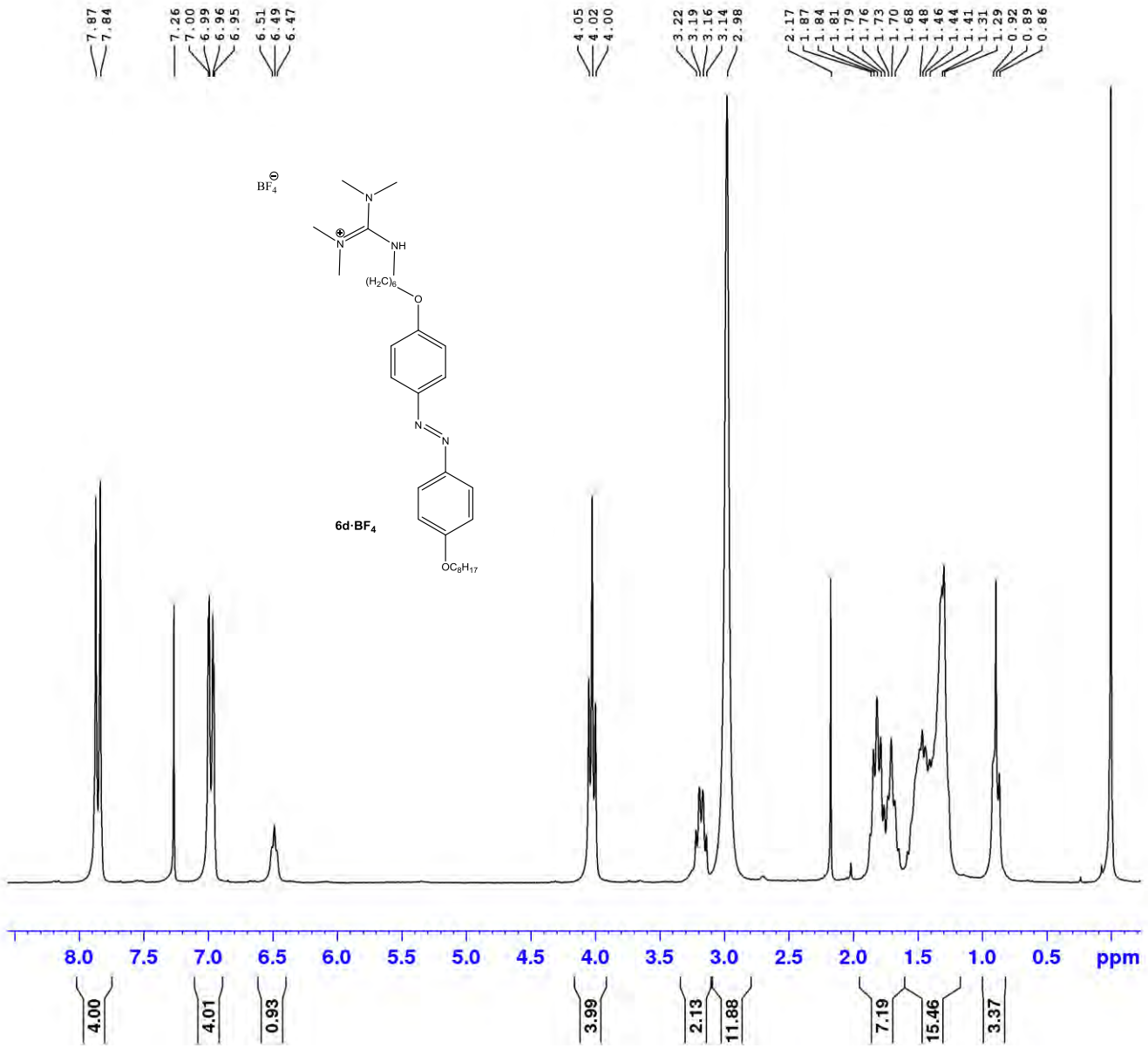
Analysis Info

Analysis Name	Laschat-Wuckert WUK 1065_12_01_22992.d	Acquisition Date	05.02.2014 09:13:41
Method	loop-tune-low-negativ.m	Operator	wo/tri
Sample Name	Laschat-Wuckert WUK 1065	Instrument	micrOTOF-Q 43
Comment			

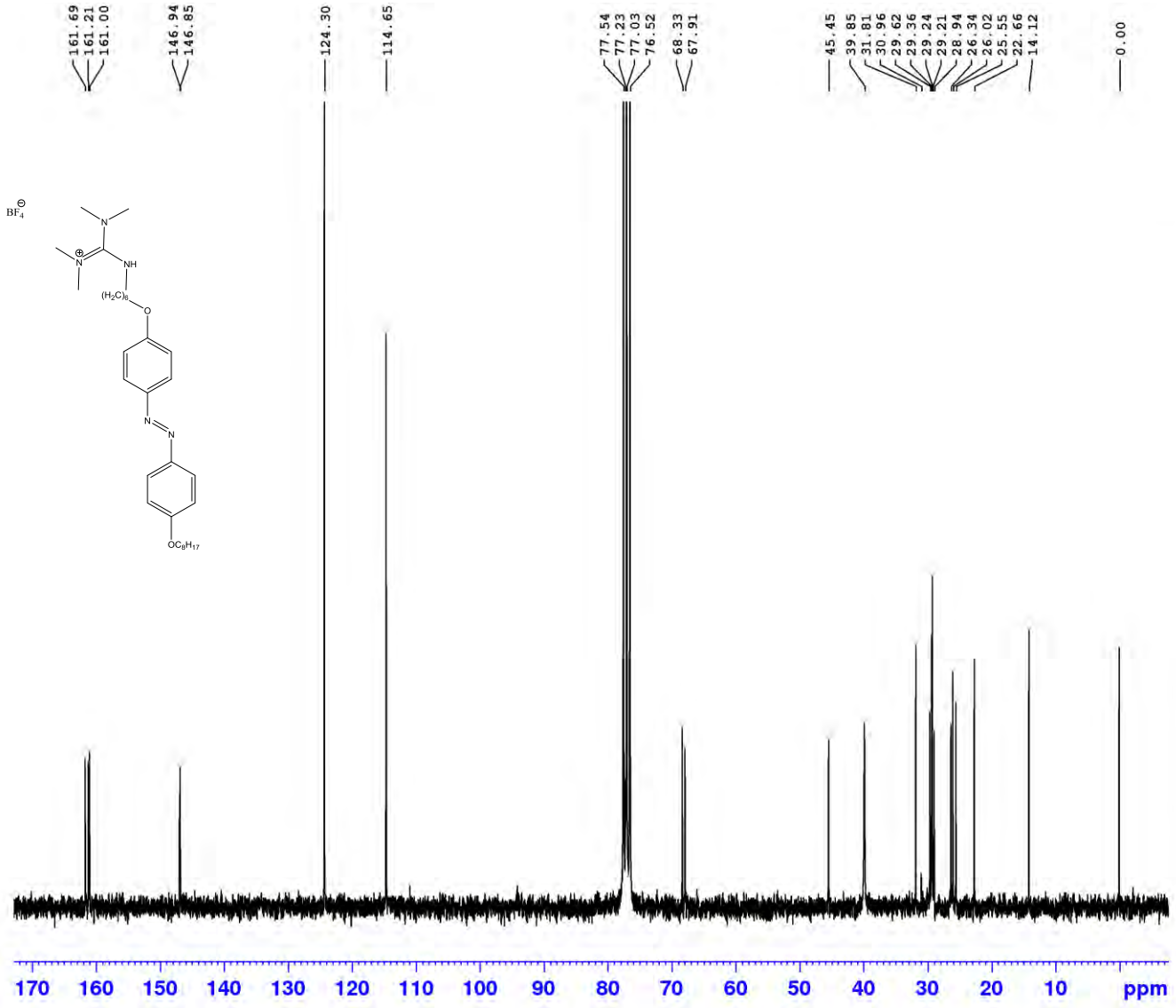
Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.8 Bar
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



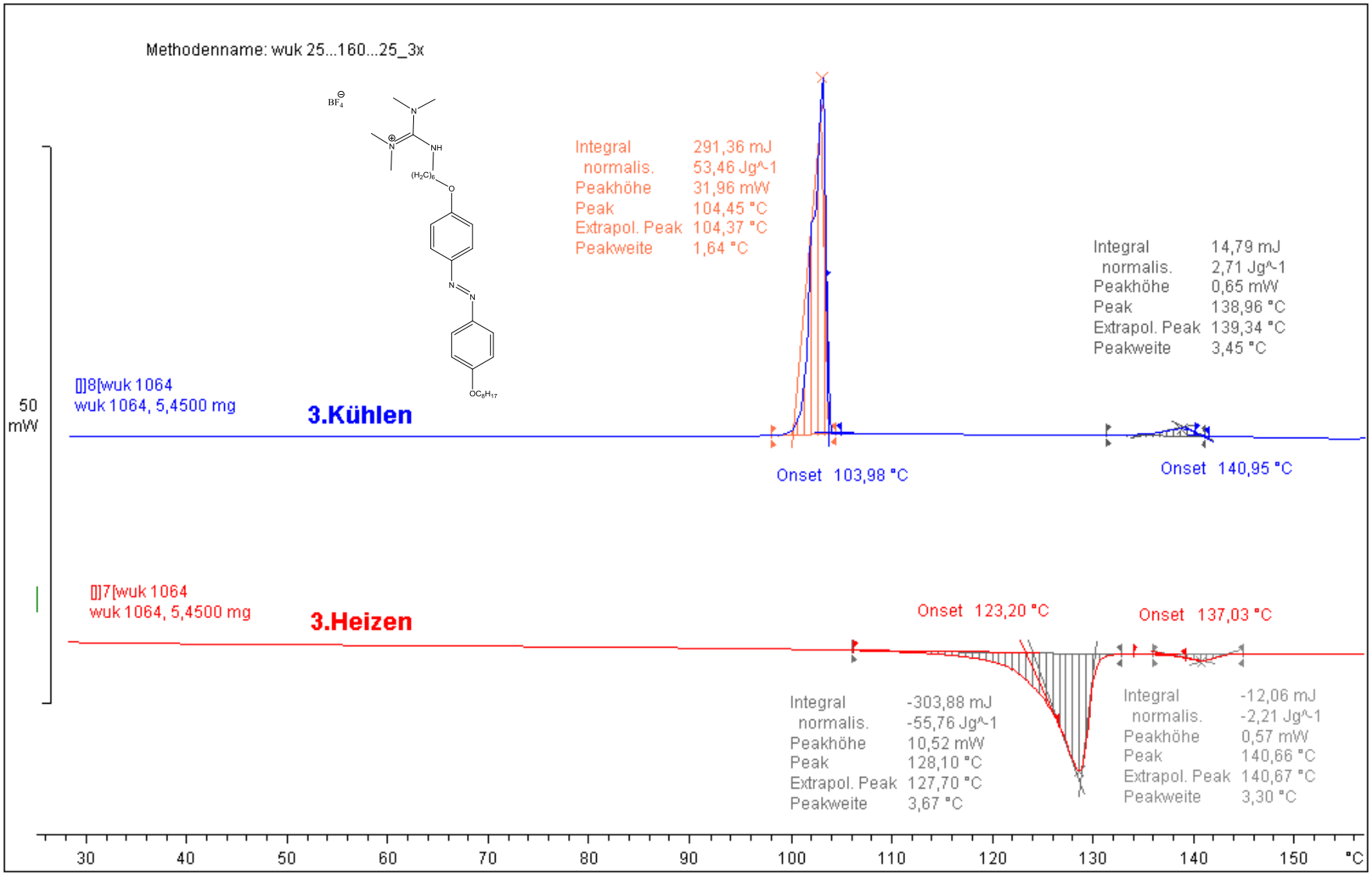



```
Current Data Parameters
NAME                  Jan31-2014
EXPNO                        410
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20140203
Time                        8.09
INSTRUM                    spect
PROBHD    5 mm QNP 1H/13
PULPROG                     zg30
TD                         65536
SOLVENT                    CDCl3
NS                            64
DS                             2
SWH                    5175.983 Hz
FIDRES                 0.078979 Hz
AQ                     6.3307776 sec
RG                         228.1
DW                        96.600 usec
DE                         8.00 usec
TE                         300.0 K
D1                    1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                        10.40 usec
PL1                       -6.00 dB
SFO1                250.1315447 MHz

F2 - Processing parameters
SI                         65536
SF                 250.1300062 MHz
WDW                           EM
SSB                0
LB                         0.30 Hz
GB                 0
PC                         1.00
```



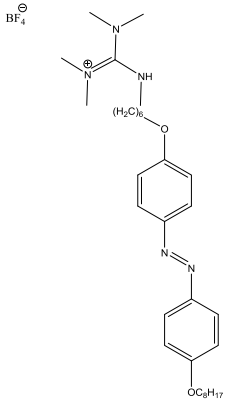

```
Current Data Parameters
NAME                  Jan31-2014
EXPNO                        411
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20140201
Time                       13.02
INSTRUM                    spect
PROBHD   5 mm QNP 1H/13
PULPROG                  zgpg30
TD                          65536
SOLVENT                     CDCl3
NS                           3072
DS                              4
SWH                  15060.241 Hz
FIDRES                0.229801 Hz
AQ                    2.1757953 sec
RG                           2048
DW                         33.200 usec
DE                          8.00 usec
TE                         300.0 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                             1

======== CHANNEL f1 ========
NUC1                         13C
P1                         11.70 usec
PL1        0 dB
SFO1                62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                         1H
PCPD2                    100.00 usec
PL2                       -6.00 dB
PL12                      18.50 dB
PL13                      15.00 dB
SFO2               250.1310005 MHz

F2 - Processing parameters
SI                           32768
SF                  62.8952403 MHz
WDW                             EM
SSB        0
LB                         1.00 Hz
GB         0
PC                         1.40
```

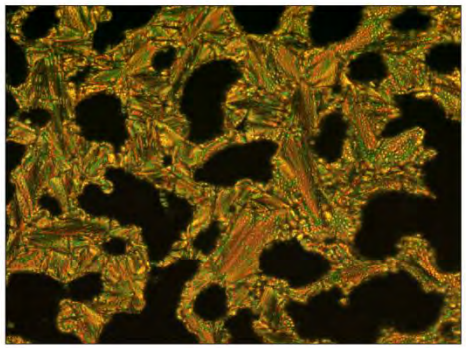
^exo wuk 1064_3.Lauf 18.09.2014 15:50:21



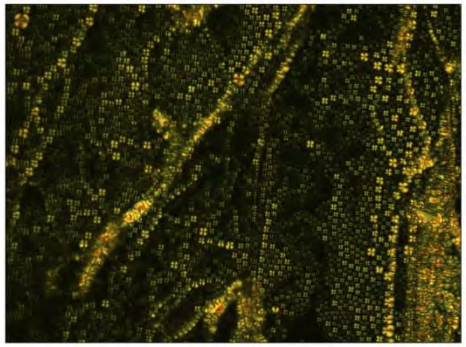
Uni Stuttgart - AK Laschat: Wuckert METTLER TOLEDO STAR^{e} SW 7.01

8 Sp 6 Tetrafluoroborat (wuk 1064)

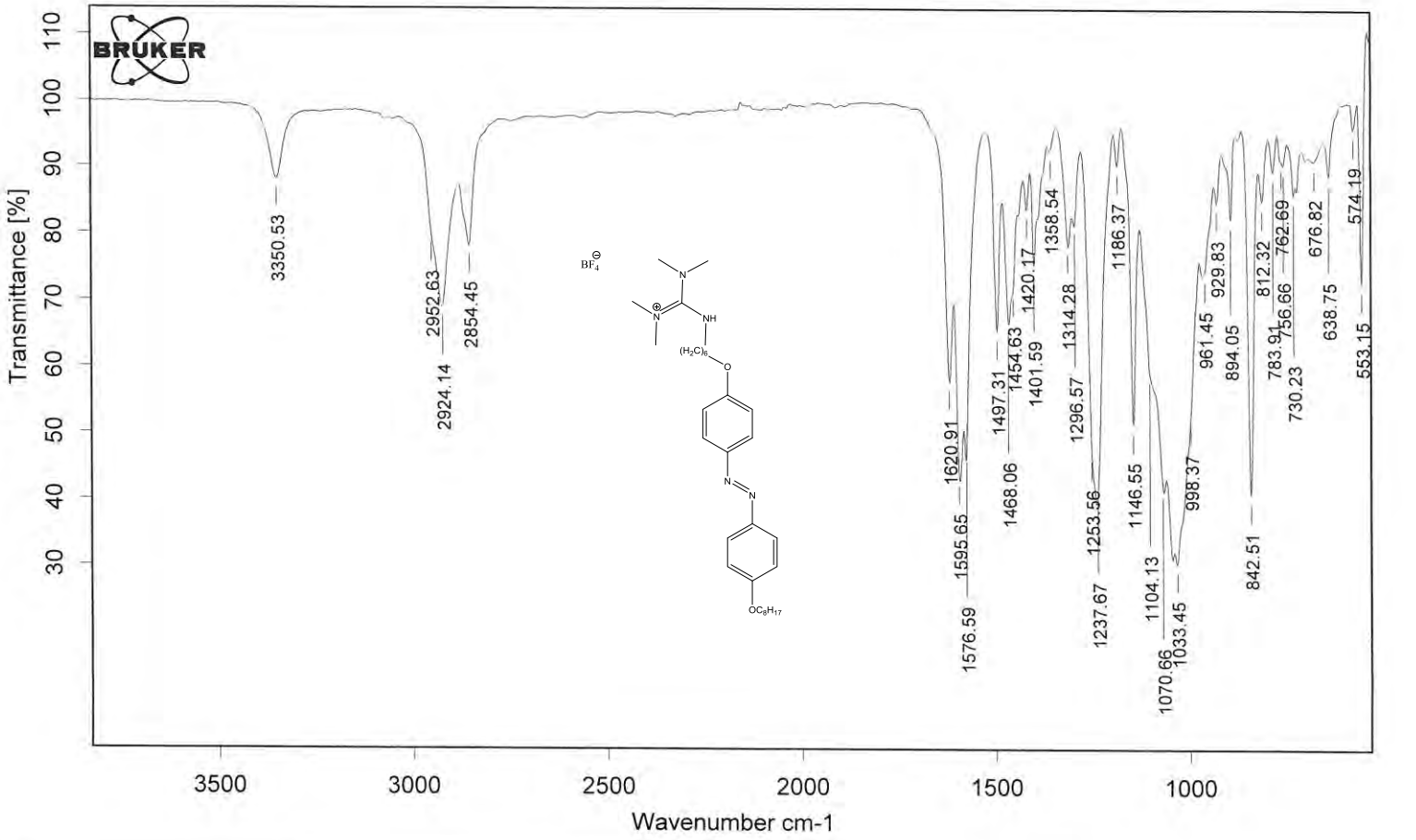




Bildname: wuk 1064.1
Bildkommentar: Kühlen von I 148° - I mit 10°/min
bei 140°
200x



Bildname: wuk 1064.2
Bildkommentar: Heizen
142
200x



D:\IR-DATEN\twiehaus\1064.0	Wuckert/1064	fest	31/01/2014

Wuckert

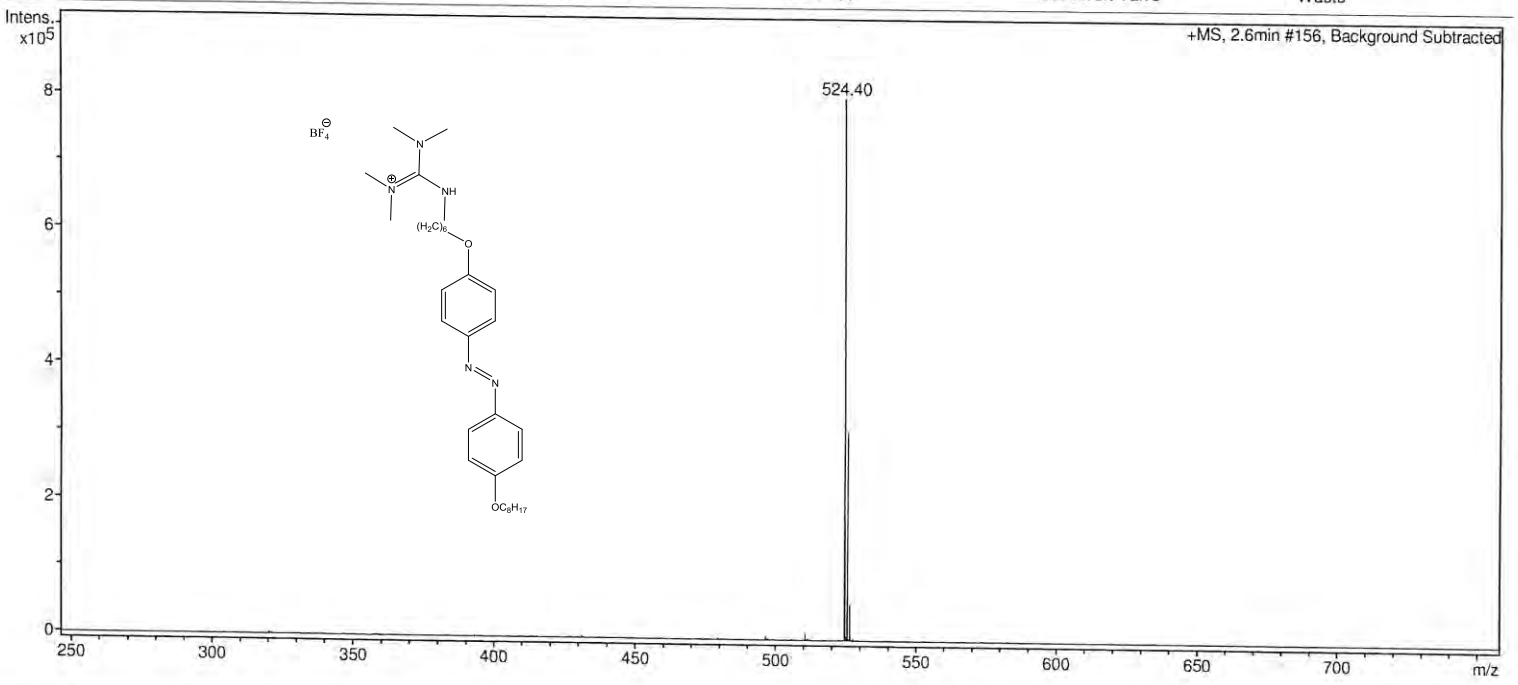
Massenspektrometrie - Universität Stuttgart

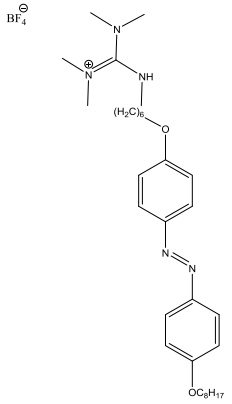
Analysis Info

Analysis Name	Laschat-Wuckert WUK 1064_11_01_22986.d	Acquisition Date	05.02.2014 08:36:32
Method	test-withloop.m	Operator	wo/tri
Sample Name	Laschat-Wuckert WUK 1064	Instrument	micrOTOF-Q 43
Comment			

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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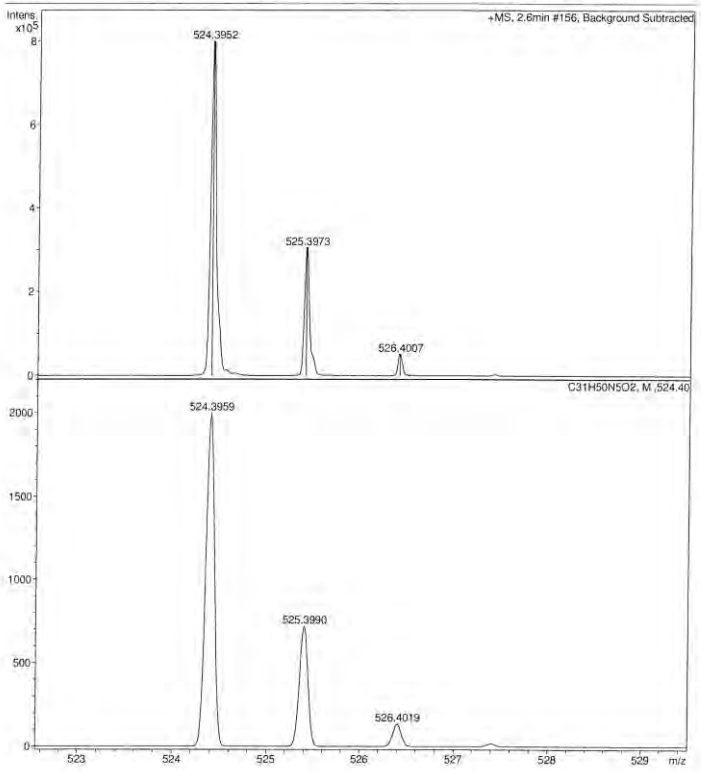
Analysis Info

Analysis Name	Laschat-Wuckert WUK 1064_11_01_22986.d	Acquisition Date	05.02.2014 08:36:32
Method	test-withloop.m	Operator	wo/tri
Sample Name	Laschat-Wuckert WUK 1064	Instrument	micrOTOF-Q 43
Comment			

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



U-dc-1

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Analysis Info

Analysis Name	Laschat-Wuckert WUK 1064_11_01_22991.d	Acquisition Date	05.02.2014 09:07:33
Method	loop-tune-low-negativ.m	Operator	wo/tri
Sample Name	Laschat-Wuckert WUK 1064	Instrument	micrOTOF-Q 43
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Negative	Set Nebulizer	0.8 Bar
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