

Comparison of a nucleosidic vs. non-nucleosidic postsynthetic “Click” modification of DNA with base-labile fluorescent probes

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Supporting Information

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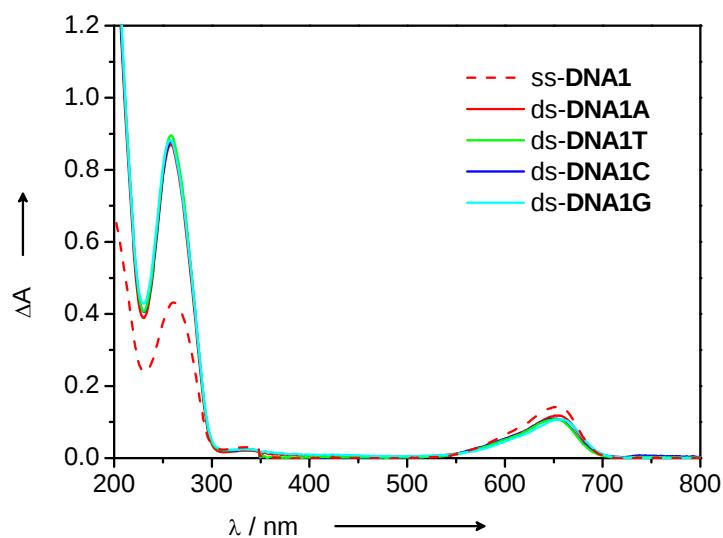
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Figure S1

UV/Vis absorption spectra of the single strand **DNA1** and the corresponding duplex set (2.5 μM) in sodium phosphate buffer (10 mM) of pH 7.0, NaCl (250 mM).

**Figure S2**

UV/Vis absorption spectra of single strand **DNA2** and the corresponding duplex set (2.5 μM) in sodium phosphate buffer (10 mM) of pH 7.0, NaCl (250 mM).

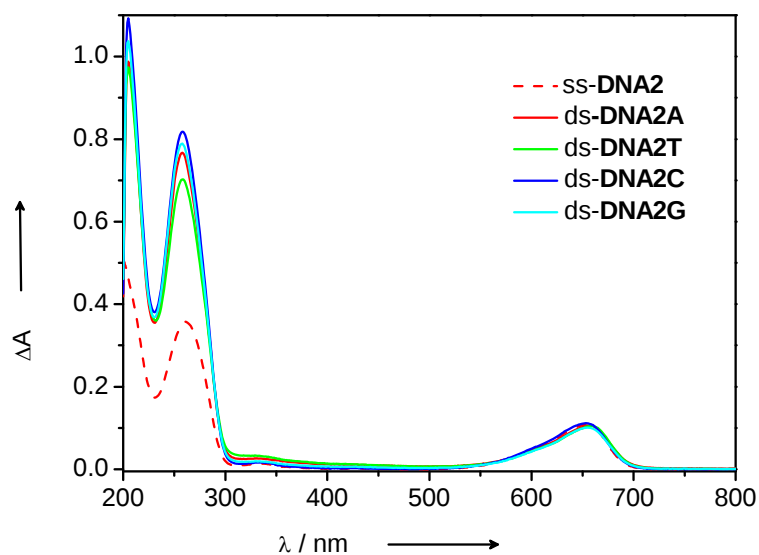
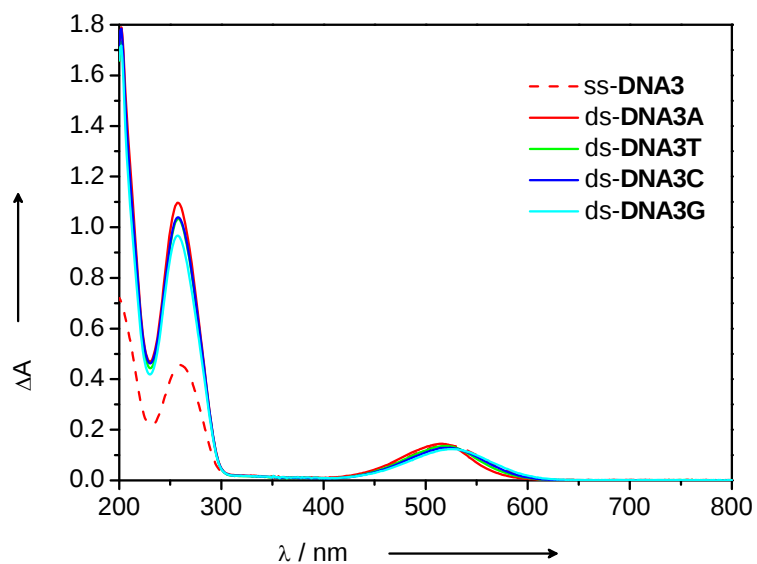


Figure S3

UV/Vis absorption spectra of single strand **DNA3** and the corresponding duplex set (2.5 μM) in sodium phosphate buffer (10 mM) of pH 7.0, NaCl (250 mM).

**Figure S4**

UV/Vis absorption spectra of single strand **DNA5** (2.5 μM) and the corresponding duplex set in sodium phosphate buffer (10 mM) of pH 7.0, NaCl (250 mM).

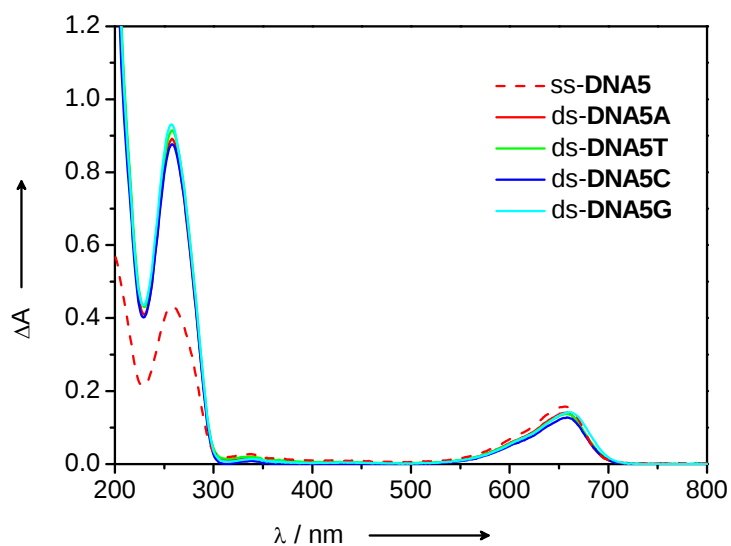
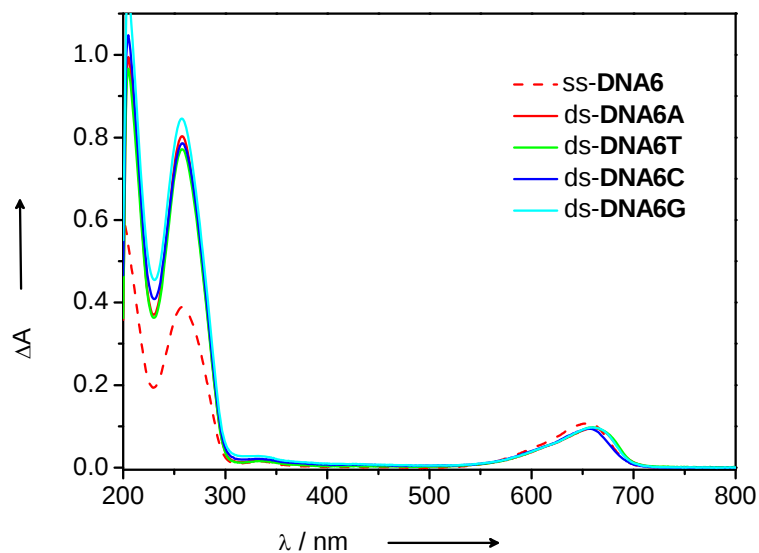
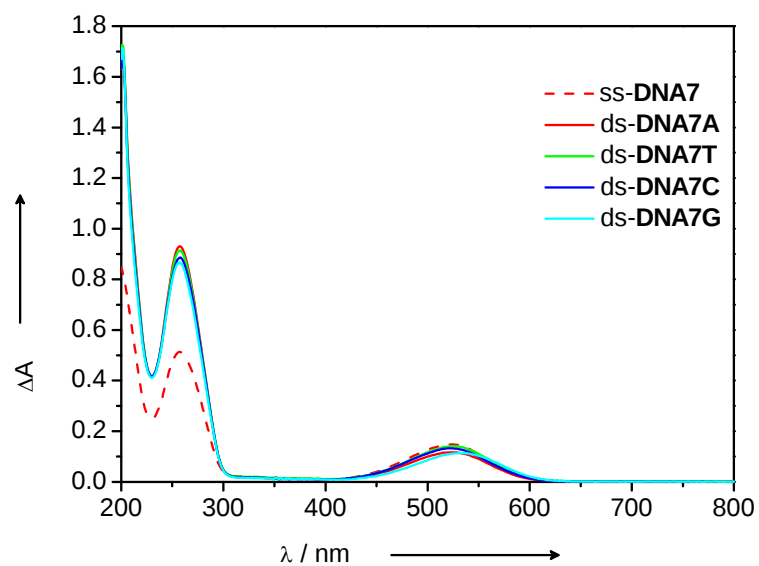


Figure S5

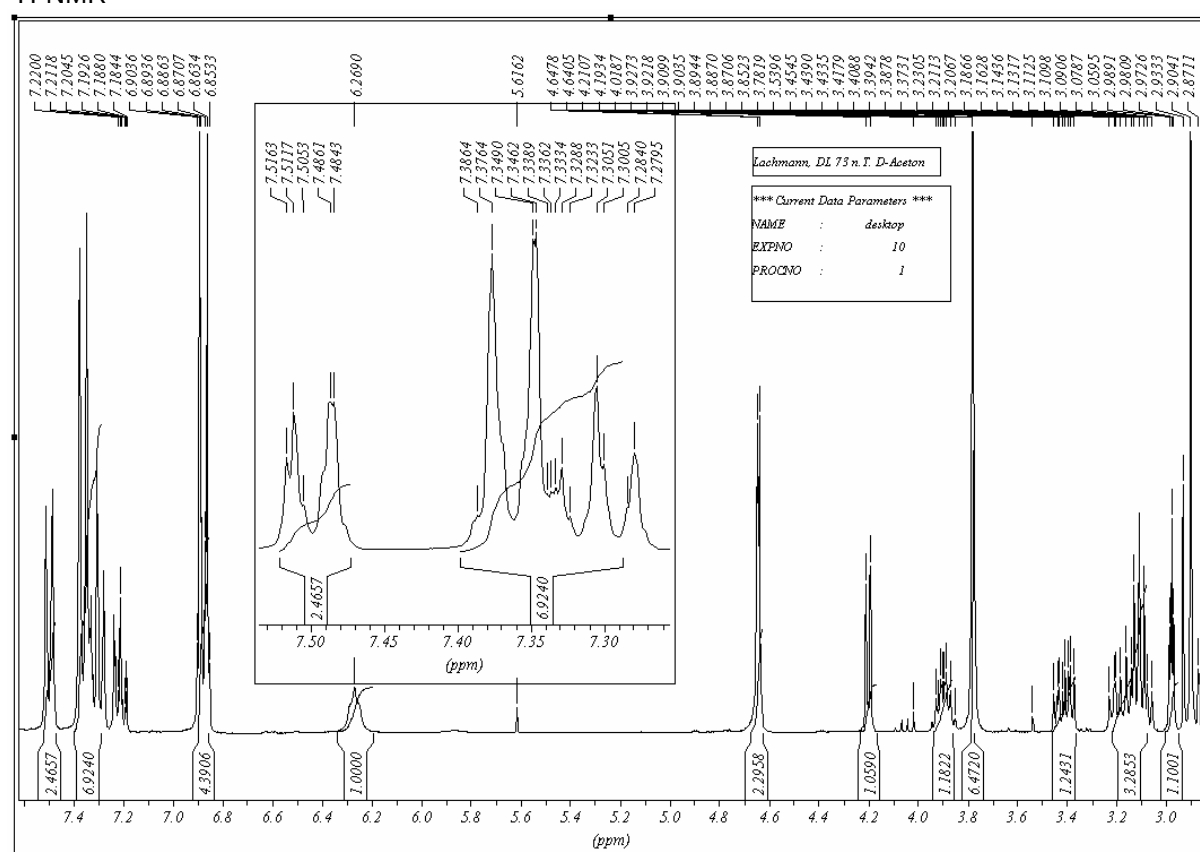
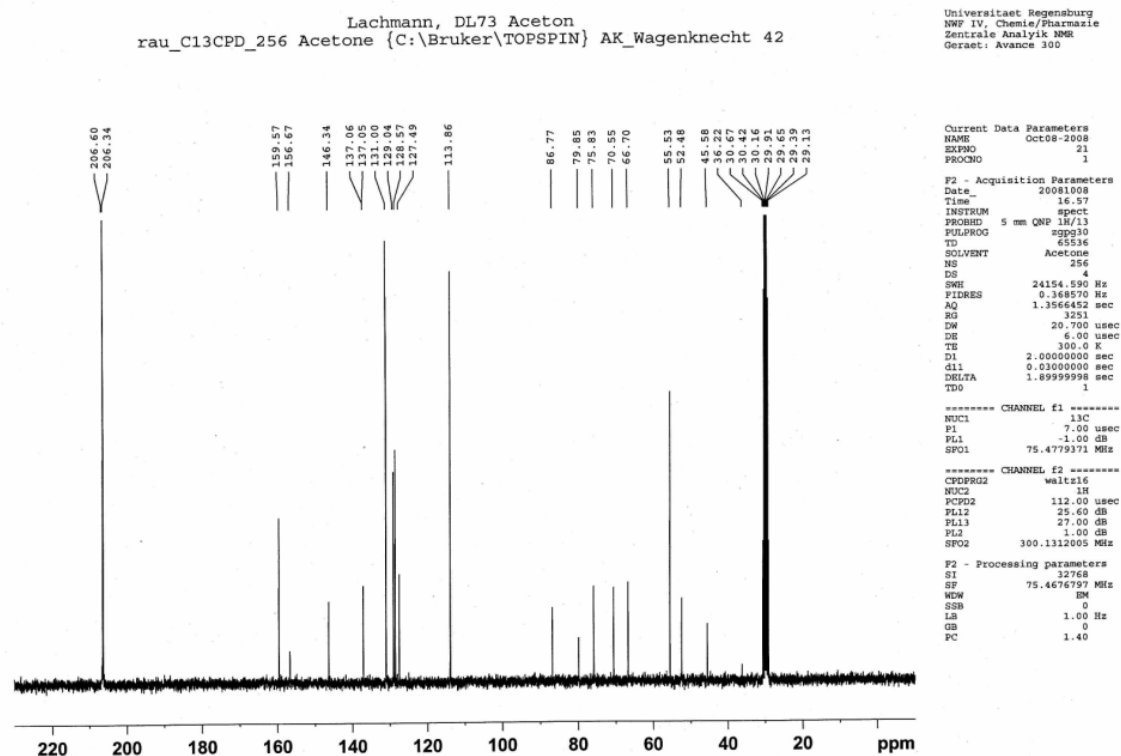
UV/Vis absorption spectra of single strand **DNA6** and the corresponding duplex set (2.5 μM) in sodium phosphate buffer (10 mM) of pH 7.0, NaCl (250 mM).

**Figure S6**

UV/Vis absorption spectra of single strand **DNA7** and the corresponding duplex set (2.5 μM) in sodium phosphate buffer (10 mM) of pH 7.0, NaCl (250 mM).



Compound 5

¹H-NMR¹³C-NMR

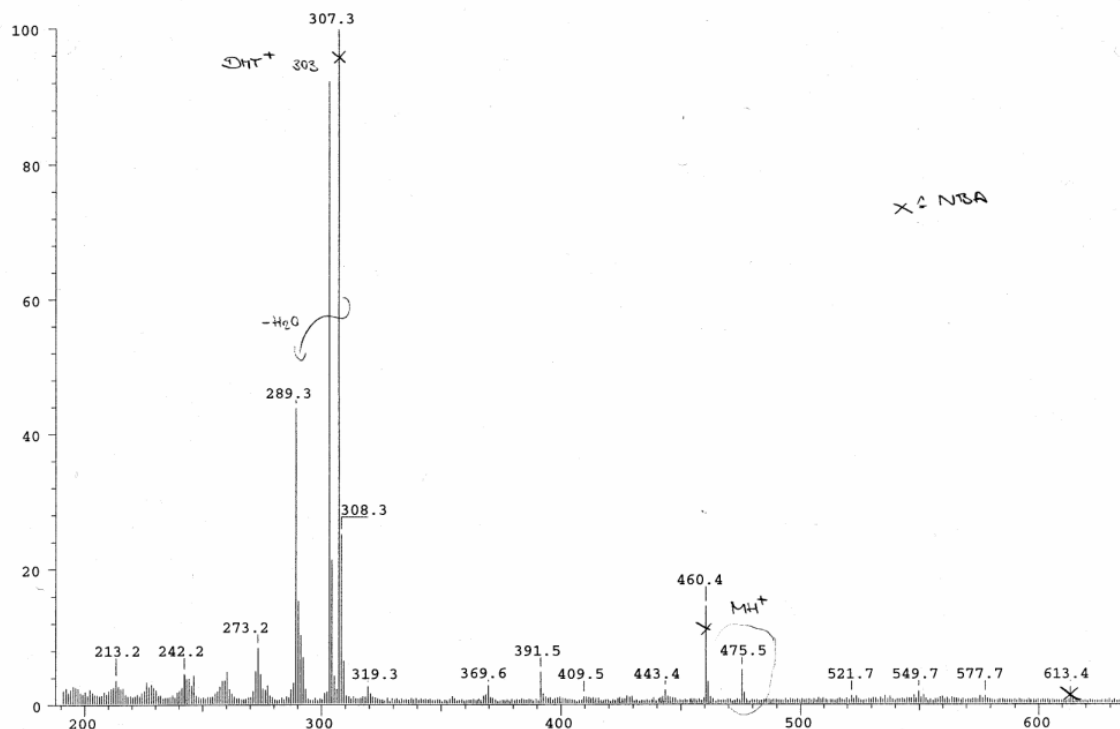
ESI-MS

SPEC: lach1 (22-Oct-08 14:58:35)

Scans: 1 > 30

REG #9 @ 1.84 min (FAB +VE +HMR BSCAN (EXP) UP LR NRM) (/25>30)

5.9E+05



HR-MS analysis:

Limit: (0)

: (160) C100.H100.N10.O10

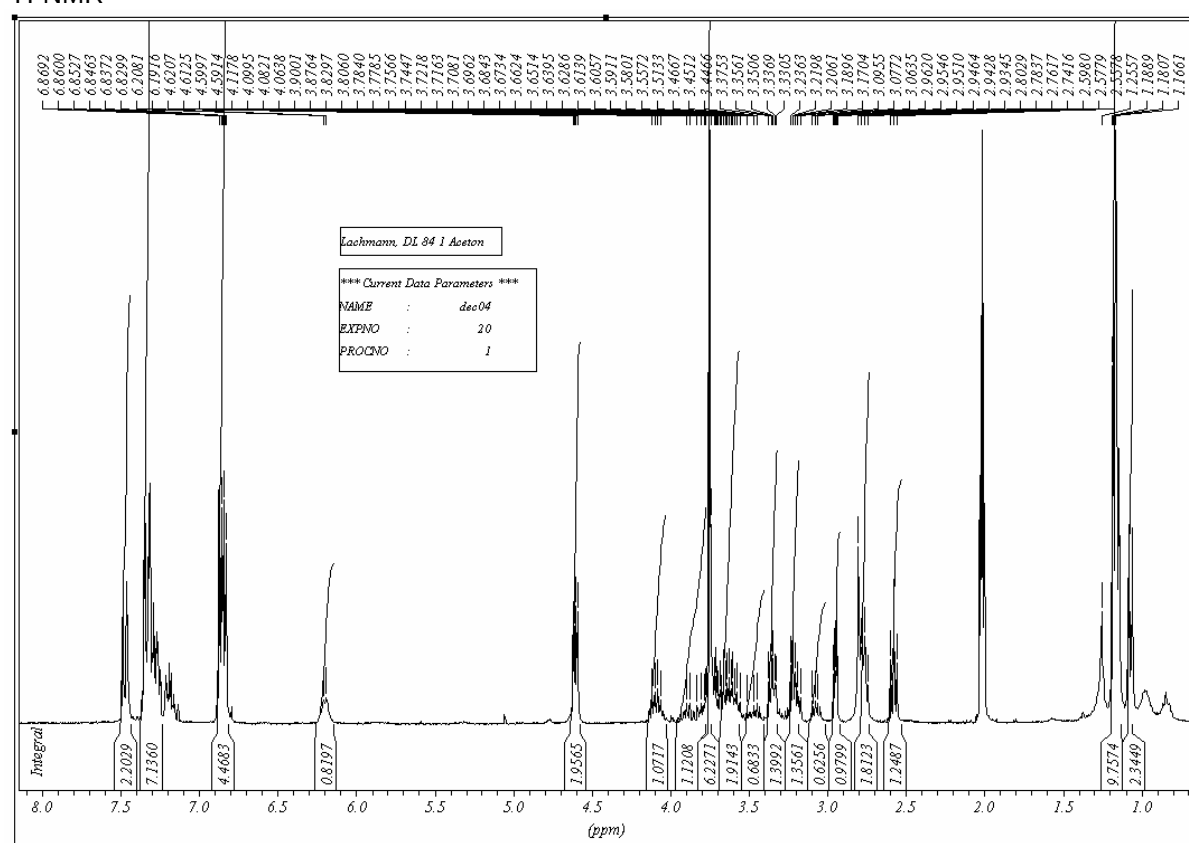
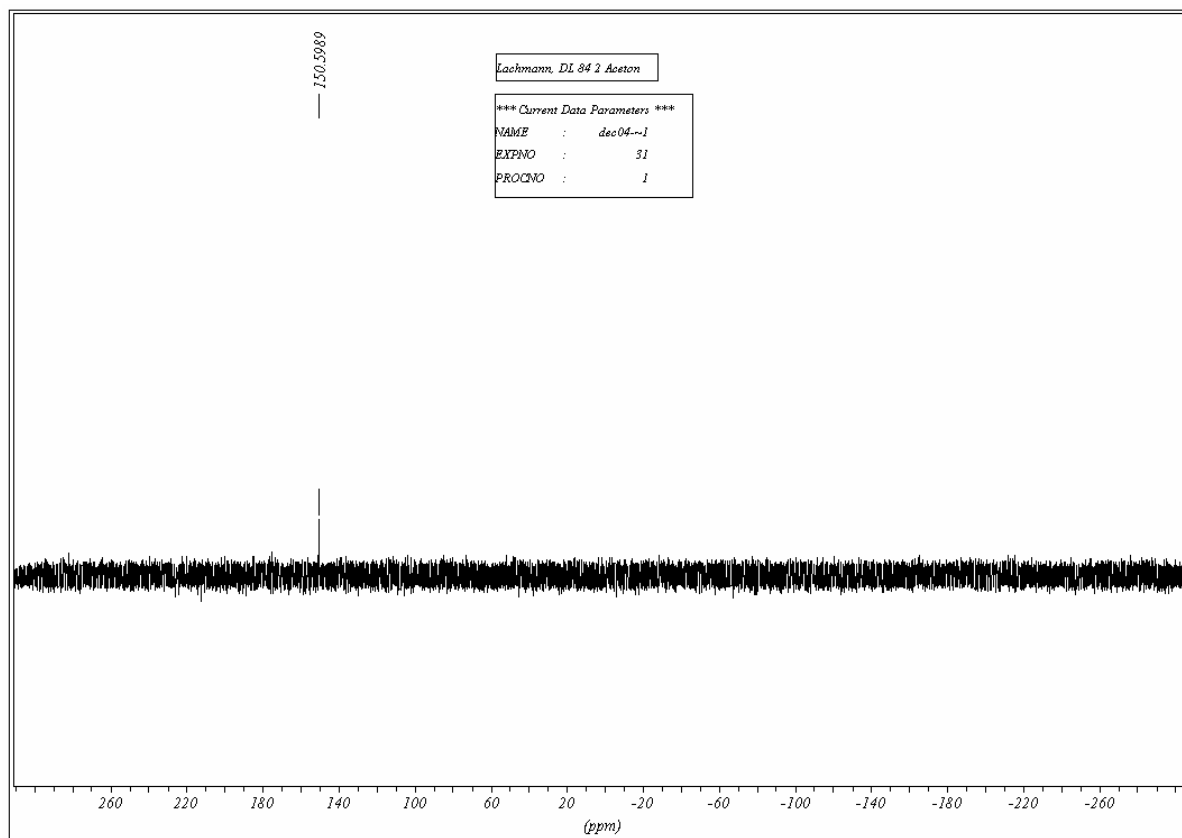
Peak: 400.00 mmu R+D: -0.5 > 50.0

Mass of (476.2085) = 476.208500000 (found) PI-LSIMS

Abs Abun. .7153375745

Delta (ppm)	R+	Formula
.314946	19.5	C29.H26.N5.O2
1.38099	7.0	C15.H28.N10.O8
-2.4937	14.5	C28.H30.N.O6 (calcd. for C ₂₈ H ₃₀ N ₁₀ O ₆ [MH ⁺]: 476.2073)
-2.5045	20.0	C27.H24.N8.O
3.13443	19.0	C31.H28.N2.O3
4.20047	6.5	C17.H30.N7.O9
-5.3131	15.0	C26.H28.N4.O5
7.01995	6.0	C19.H32.N4.O10
-8.1217	10.0	C25.H32.O9
-8.1326	15.5	C24.H26.N7.O4
8.76251	23.5	C34.H26.N3
9.8286	11.0	C20.H28.N8.O6

Compound 6

¹H-NMR³¹P-NMR:

DNA1 HPLC

Sample Information

Universität Regensburg

AK Prof. Wagenknecht

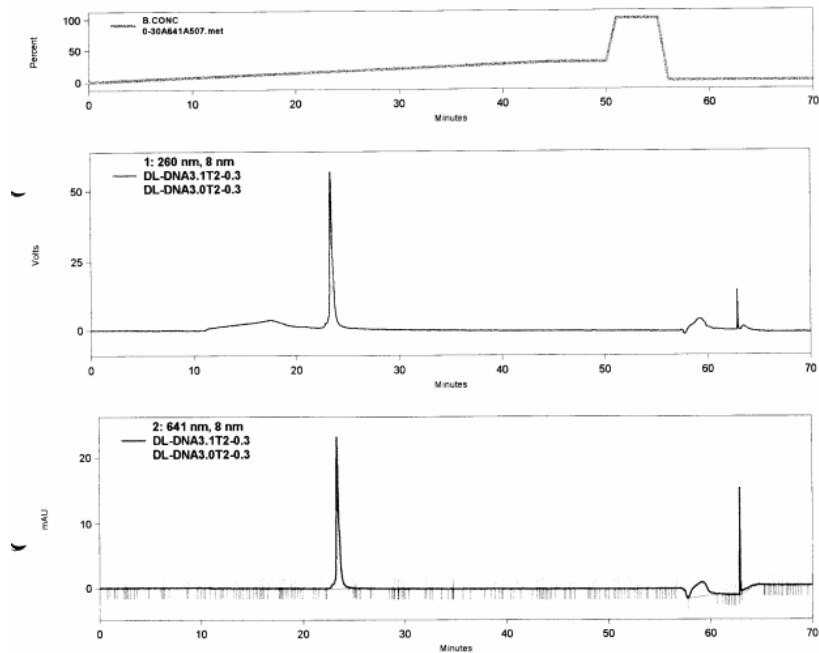
Sample Name: DL-DNA3.1T2-0.3

Injection Volume: 25 µL

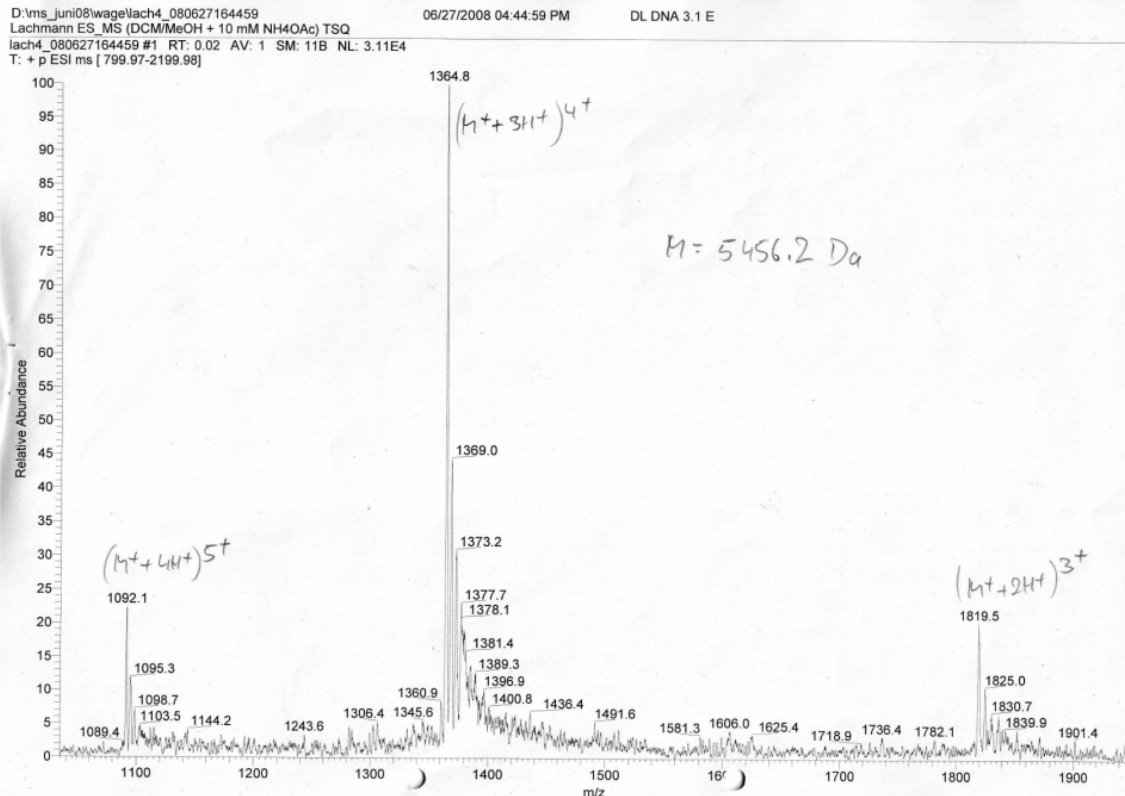
Date Acquired: 24/06/2008 21:05:01

File Name: D:\Janez\Müll\DL-DNA3.0T2-0.3

Method Name: D:\Methoden\Analytik\0-30A641A507.met



ESI-MS



DNA2 HPLC

Sample Information

Universität Regensburg

AK Prof. Wagenknecht

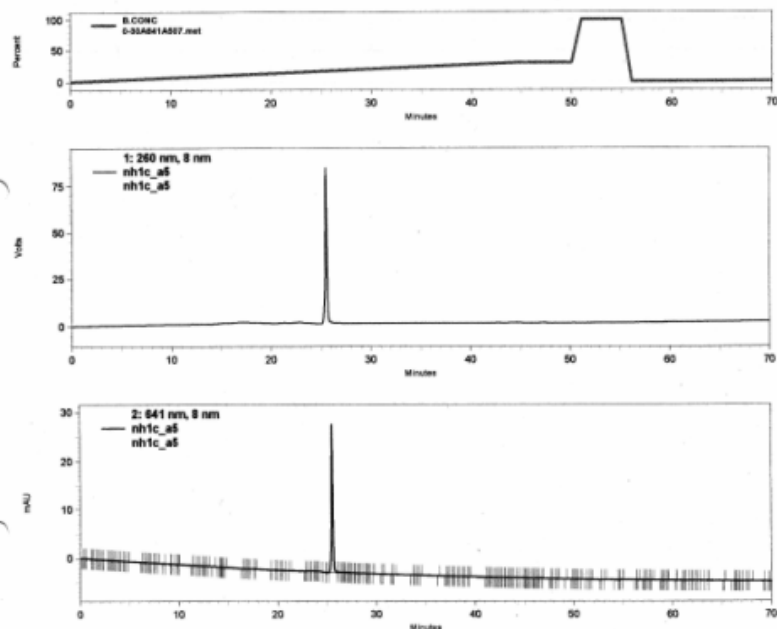
Sample Name: nh1c_a5

Injection Volume: 18 µL

Date Acquired: 22/04/2008 18:00:14

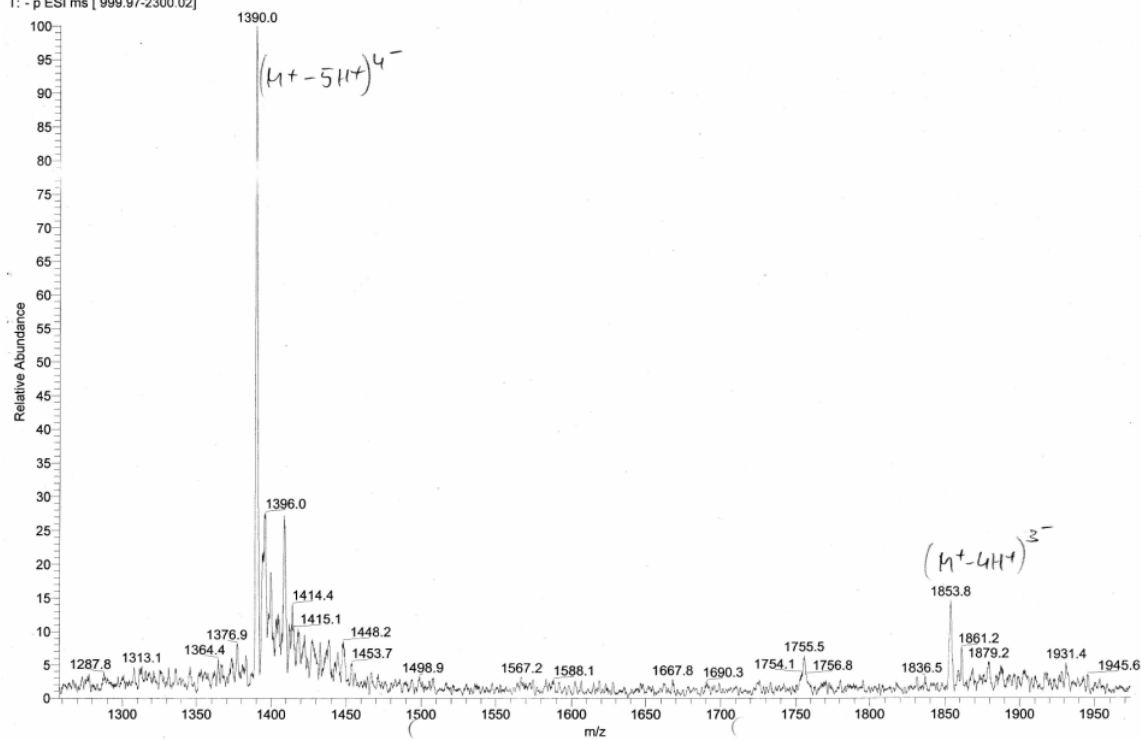
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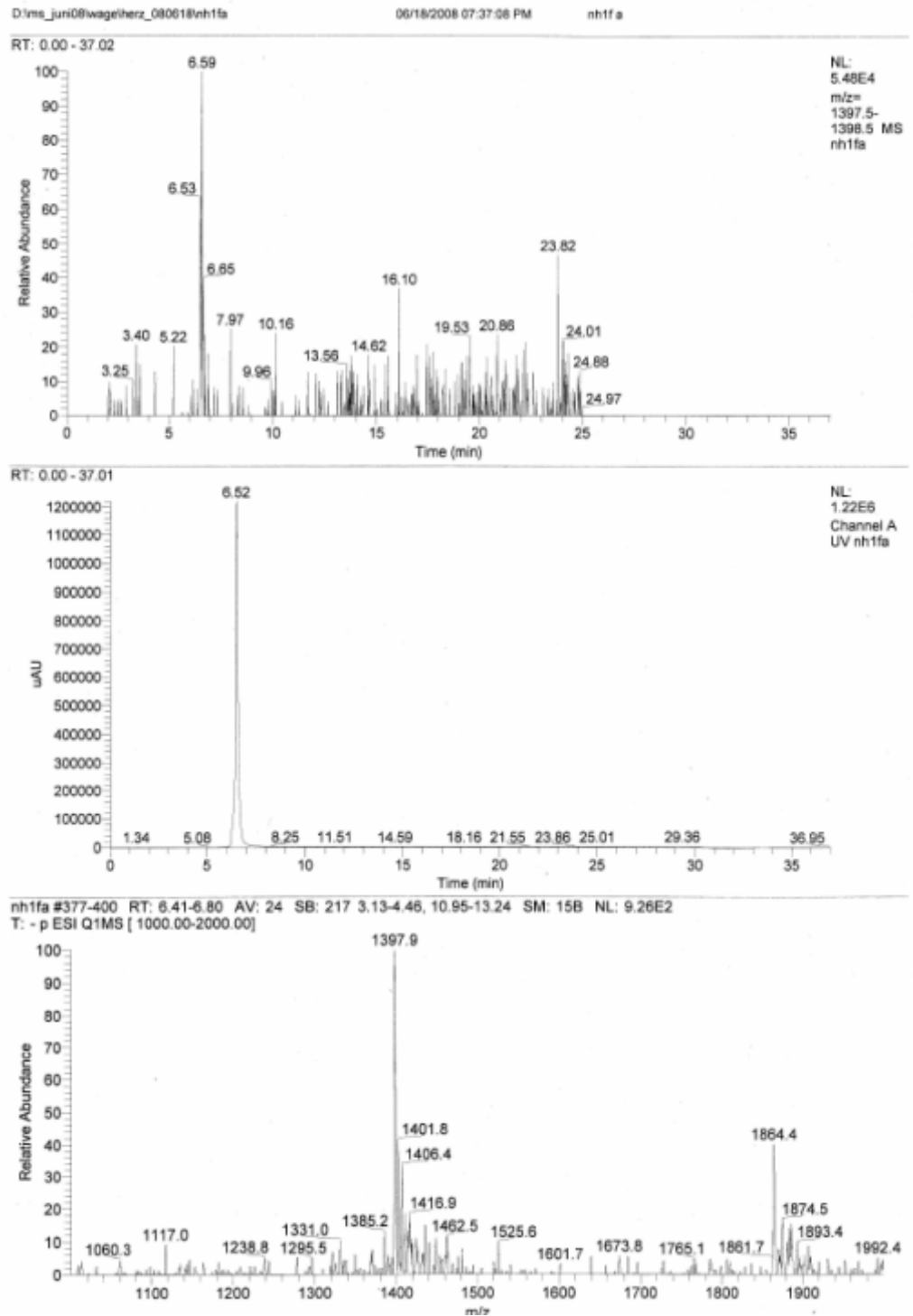
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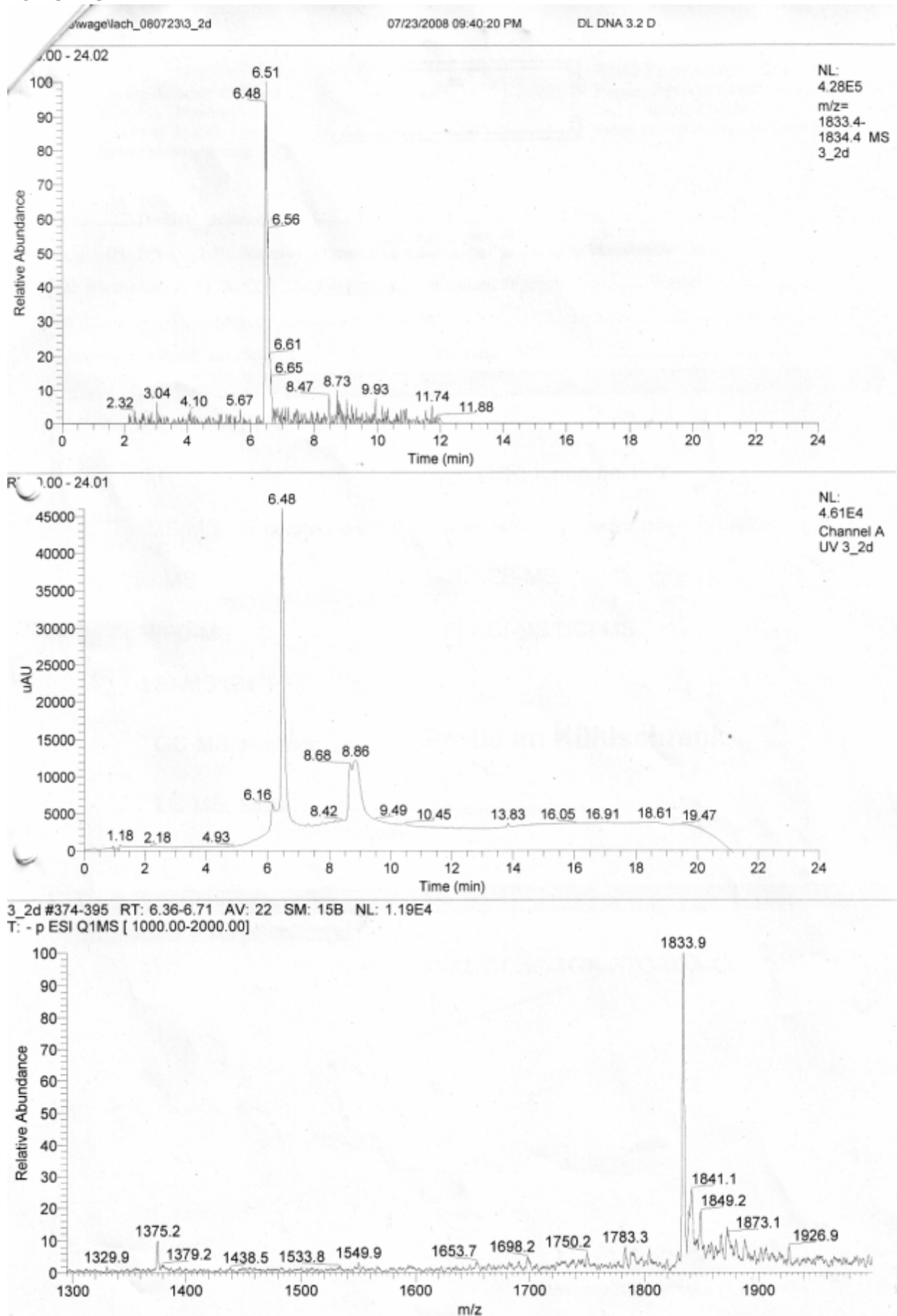


MS

D:\ms_mai\08\wage\herz41_080514123249 05/14/2008 12:32:49 PM nh1c a5
Herzig ES-MS (H₂O/MeOH + 10 mM NH₄OAc) TSQ 7000
herz41_080514123249 #1 RT: 0.02 AV: 1 SM: 11B NL: 4.87E3
T: - p ESI ms [999.97-2300.02]



DNA3
LC-ESI-MS

DNA5
LC-ESI-MS

DNA6
HPLC

Sample Information

Universität Regensburg

AK Prof. Wagenknecht

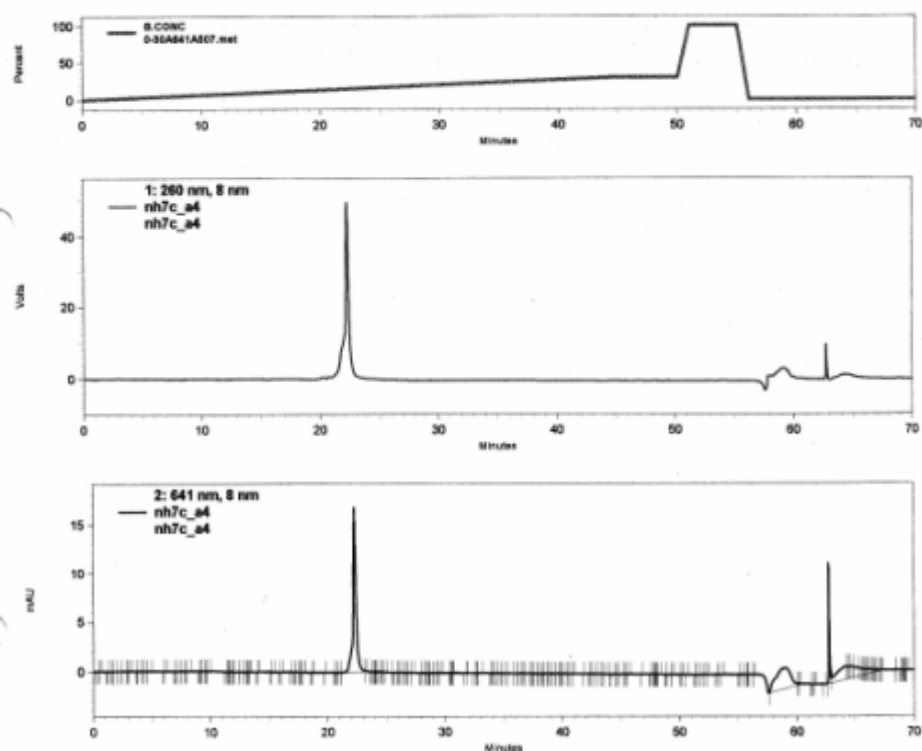
Sample Name: nh7c_a4

Injection Volume: 18 µL

Date Acquired: 23/04/2008 03:39:31

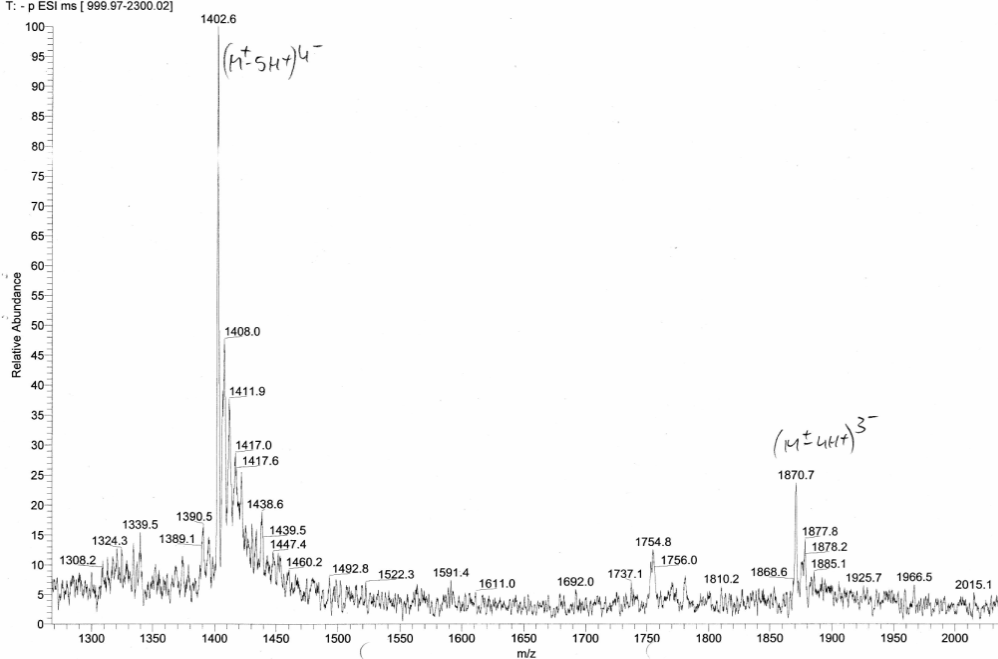
File Name: D:\Nadine\220408\nh7c_a4

Method Name: D:\Methoden\Analytik\0-30A641A507.met



D:\ms_mai08\wage\herz42
Herzig ES-MS (H₂O/MeOH + 10 mM NH₄OAc) TSQ 7000
herz42 #1 RT: 0.01 AV: 1 SM: 11B NL: 4.24E3
T: -p ESI ms [999.97-2300.02]

05/14/2008 12:44:50 PM nh7c a5



DNA7
LC-MS