# Observation of the Rare Chrysene Excimer

Oleg Khorev, Caroline Bösch, Markus Probst and Robert Häner*

Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, CH-3012 Bern, Switzerland
E-mail: robert.haener@ioc.unibe.ch

**SUPPORTING INFORMATION**

**1. Determination of the molar absorption coefficient (ε) of 3.**

The molar absorption coefficient (ε) was measured by standard procedures, giving a linear dependence of absorbance ($\lambda_{max}$ 365 nm) on concentration for solutions between $6.2\times10^{-5}$ and $1.24\times10^{-7}$ M in THF. The slope of the resultant line was 41402 (Figure S1).

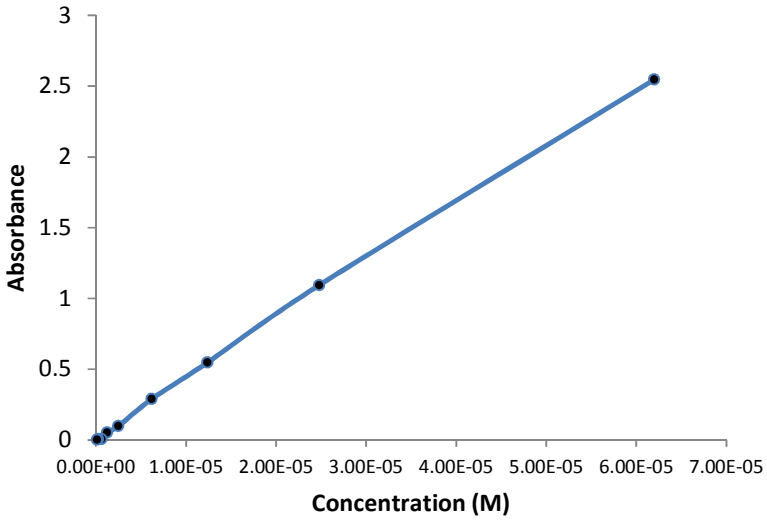


**Figure S1.** Variation of absorbance with concentration of compound **3**.

**2. Quantum yield determination.**

Quantum yields (Φ) were determined relative to 9,10-diphenylanthracene as a standard following the procedure described in the literature.[1,2]

**3. NMR spectra of compounds 3-5.**

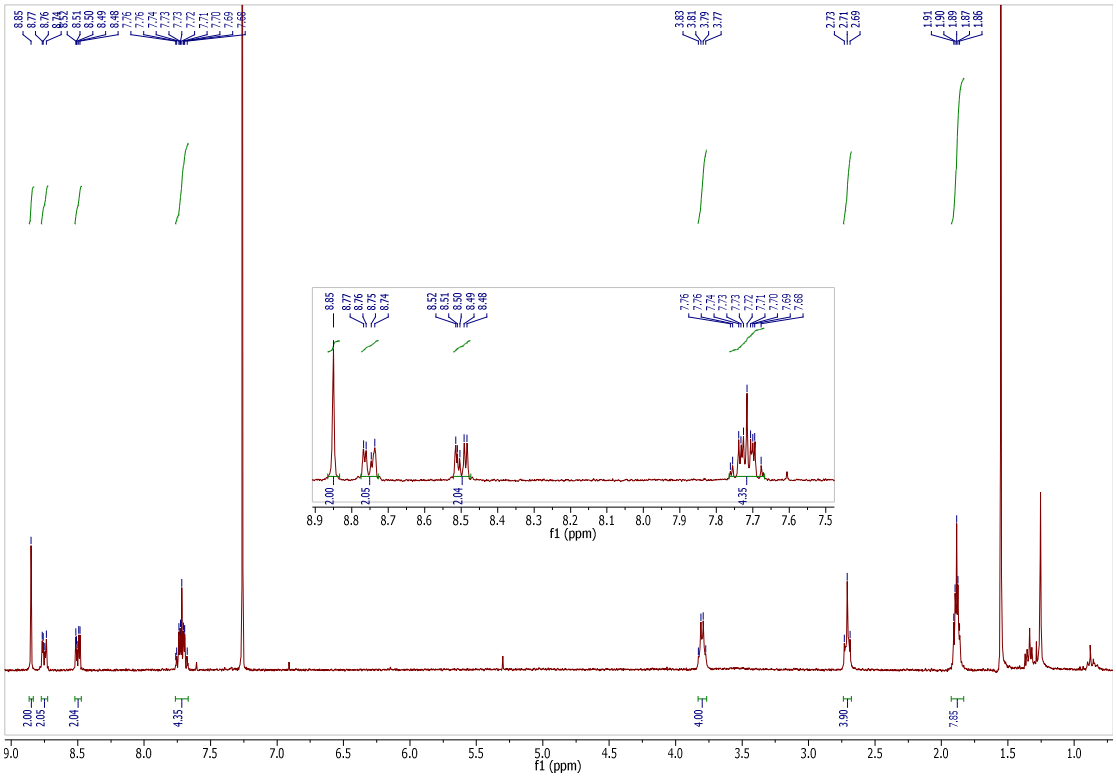


**Figure S2.** $^{1}$H NMR spectrum of compound **3** in $CDCl_3$.

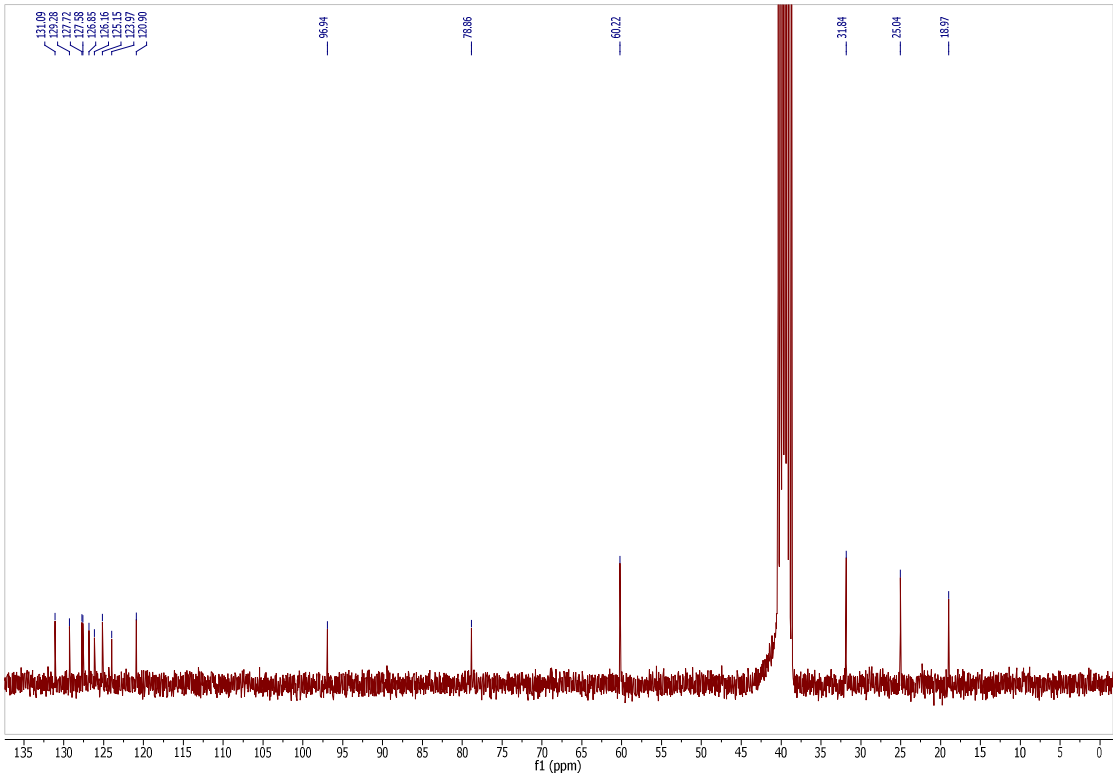


**Figure S3.** $^{13}$C NMR spectrum of compound **3** DMSO-$d_6$.

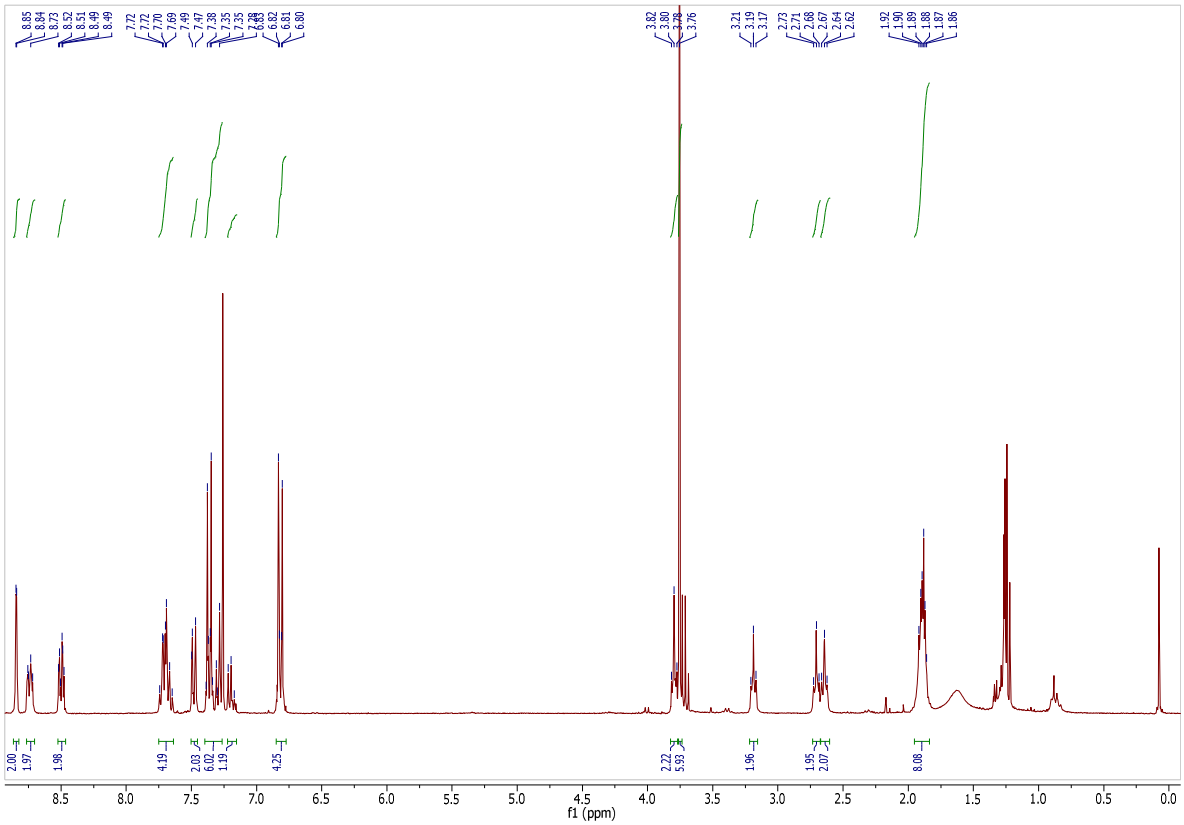


**Figure S4.** $^{1}$H NMR spectrum of compound **4** in $CDCl_3$.

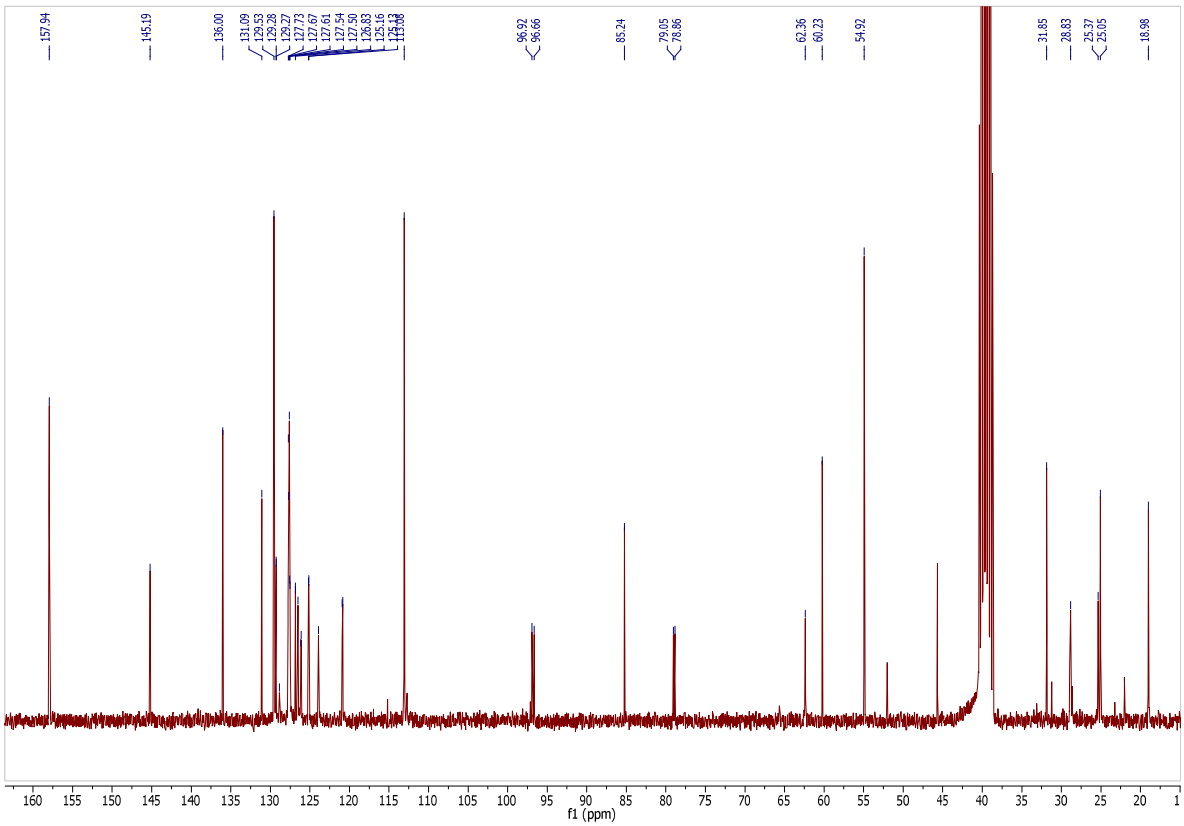


**Figure S5.** $^{13}$C NMR spectrum of compound **4** DMSO-$d_6$.

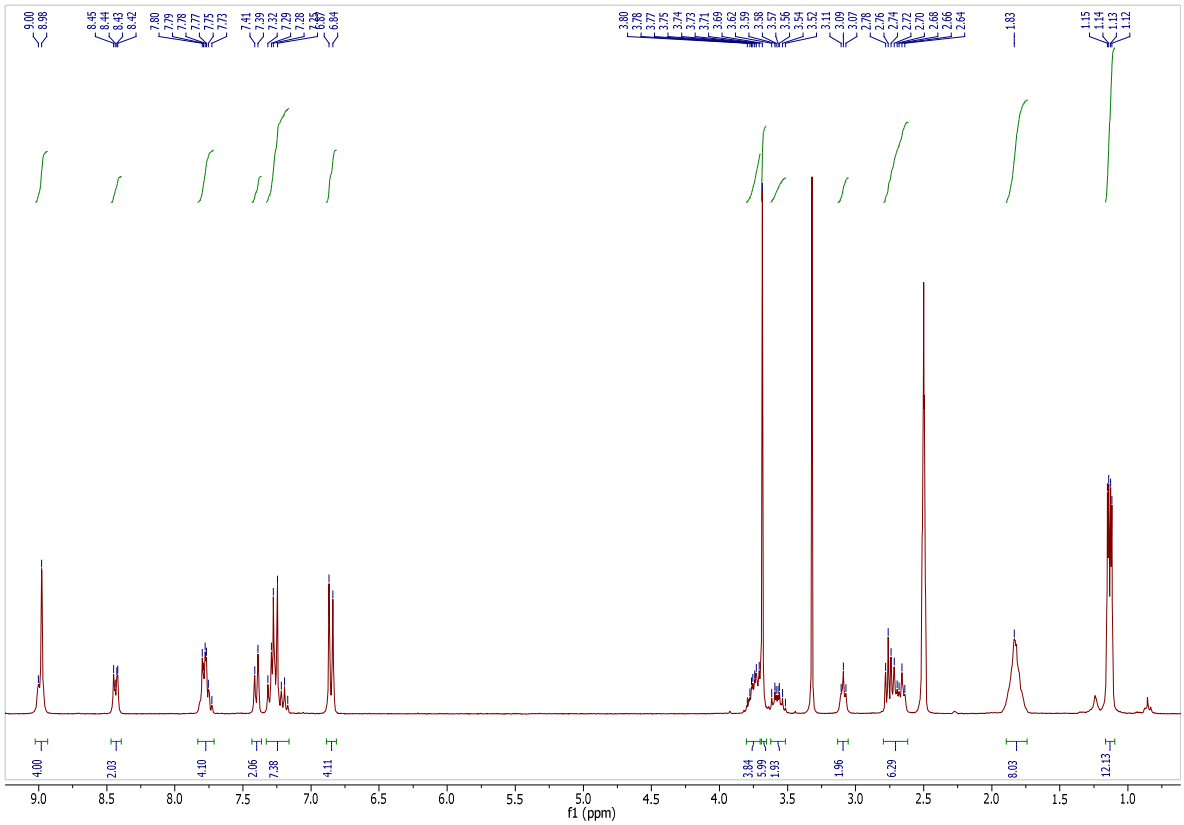


**Figure S6.** $^{1}$H NMR spectrum of compound **5** in DMSO-$d_6$.

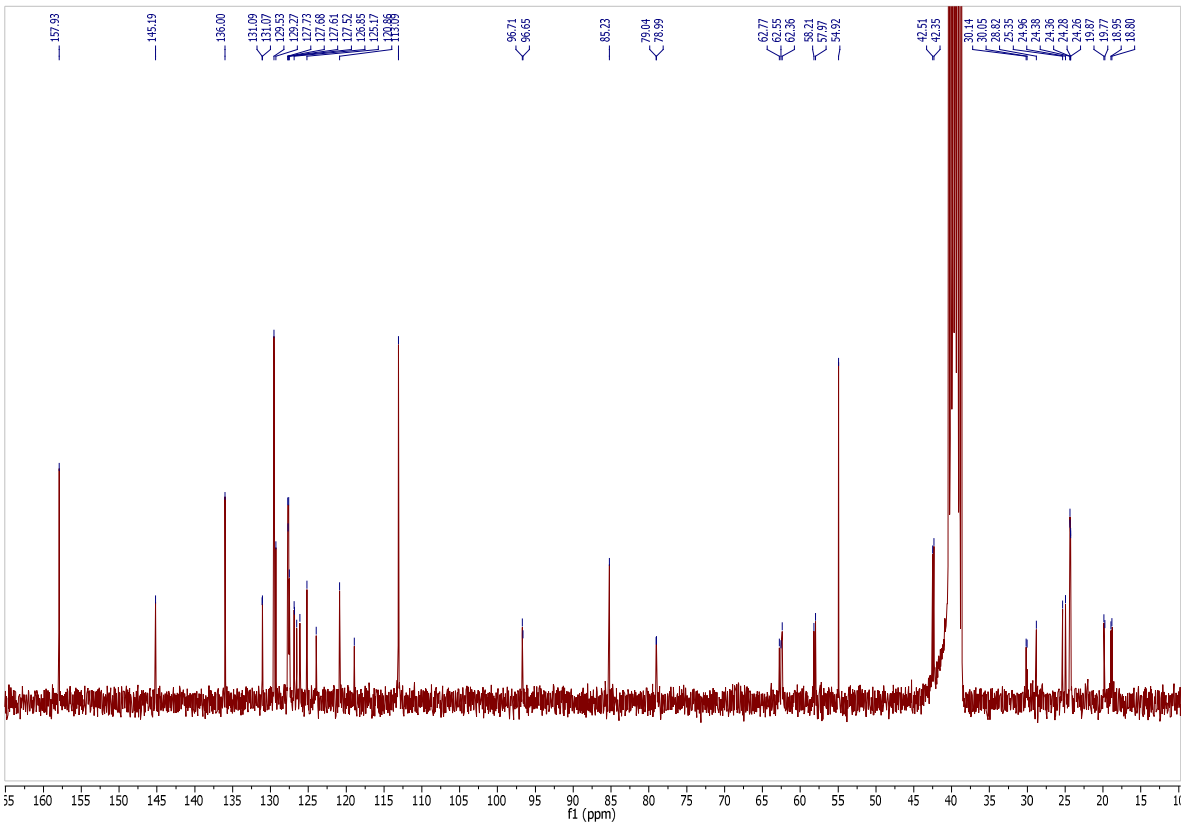


**Figure S7.** $^{13}$C NMR spectrum of compound **5** DMSO-$d_6$.

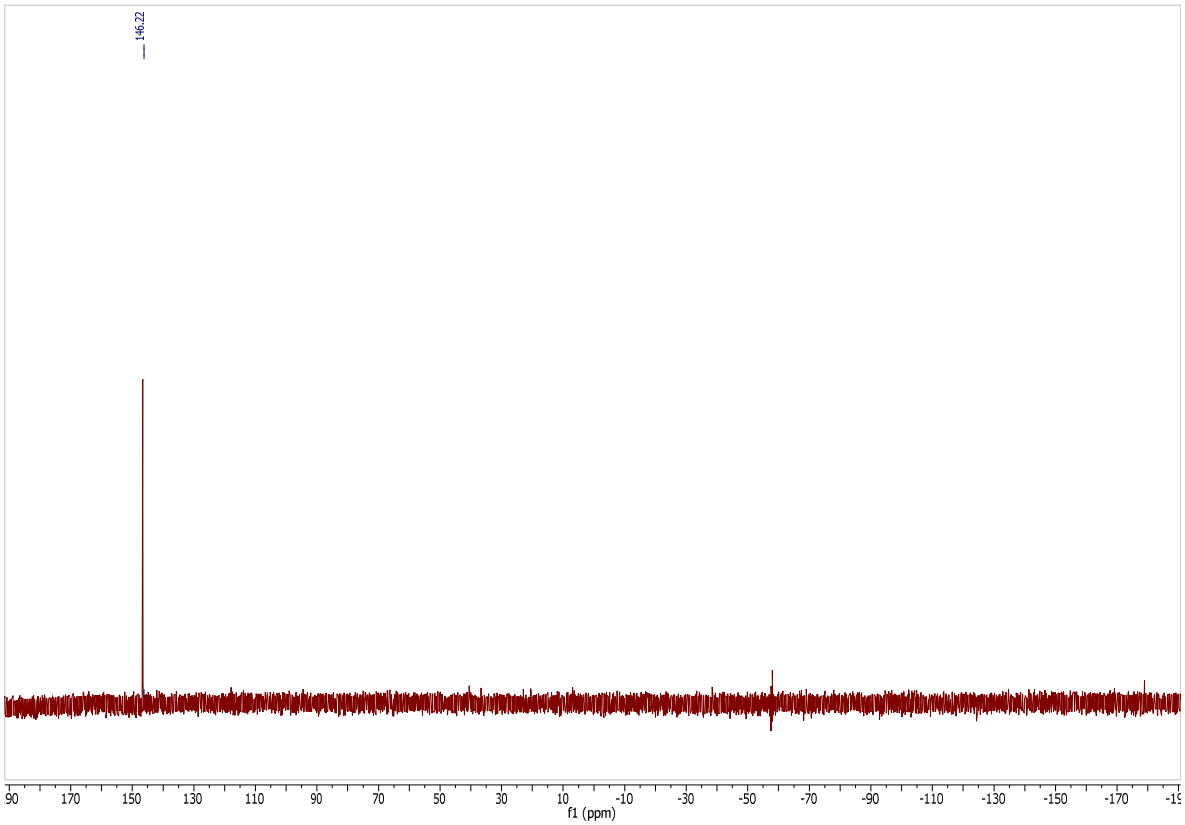


**Figure S8.** $^{31}P$ NMR spectrum of compound **5** DMSO-$d_6$.

**4. Mass spectrometry of ONs 6-9.**

Mass analysis was performed with an LTQ Orbitrap XL (Thermo Fisher Scientific, Bremen, Germany) operating at a mass resolution of 100'000 (at m/z 400). The mass spectrometer was equipped with a nano-electrospray ion source. Following HPLC purification, the lyophilised samples were dissolved in deionised water to give concentrations (per strand) of oligonucleotide **6**: 86.1 µM; oligonucleotide **7**: 151.3 µM; oligonucleotide **8**: 137 µM; oligonucleotide **9**: 168 µM. The solutions (40 µL) were diluted with an equal amount of acetonitrile/water/triethylamine (49/49/2) and 5 µl of the resultant solution were filled into a nano-electrospray needle (New Objective, Woburn, MA, USA). A potential of -750 V was applied for generation of the electrospray. Nitrogen was used as the curtain gas.

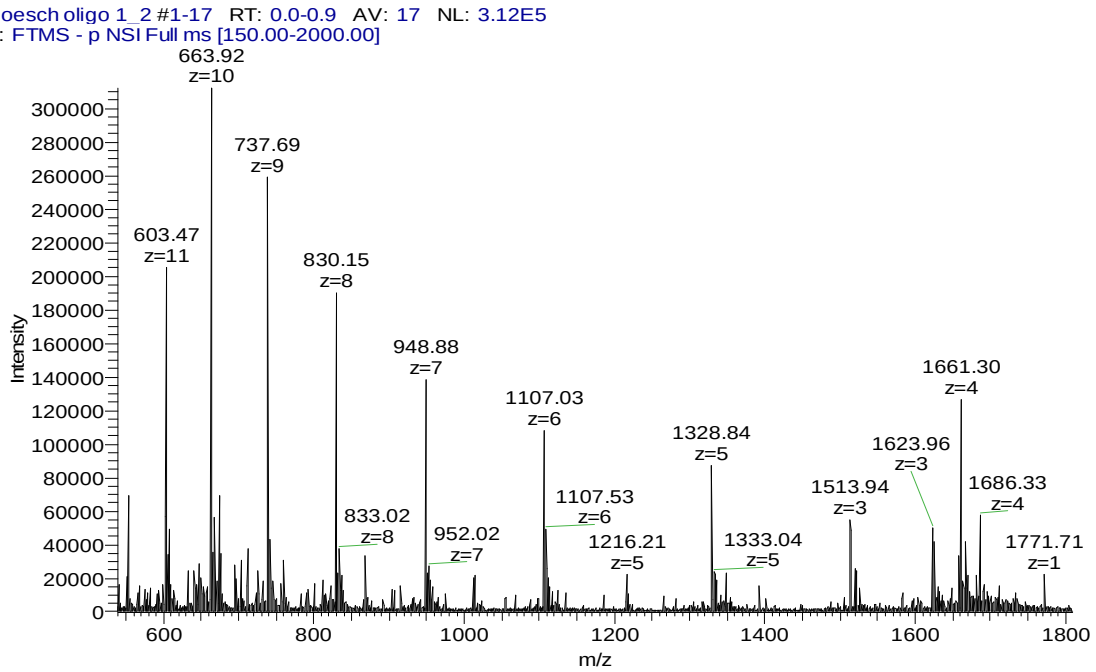


**Figure S9.** HRMS spectrum of oligonucleotide **6**.

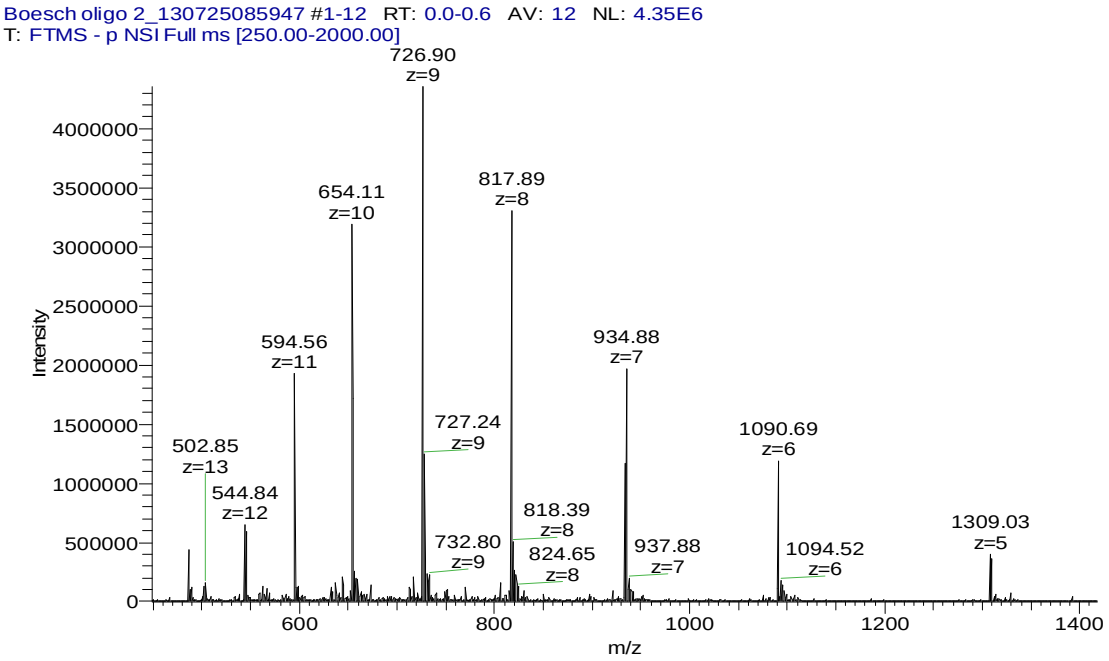


**Figure S10.** HRMS spectrum of oligonucleotide **7**.

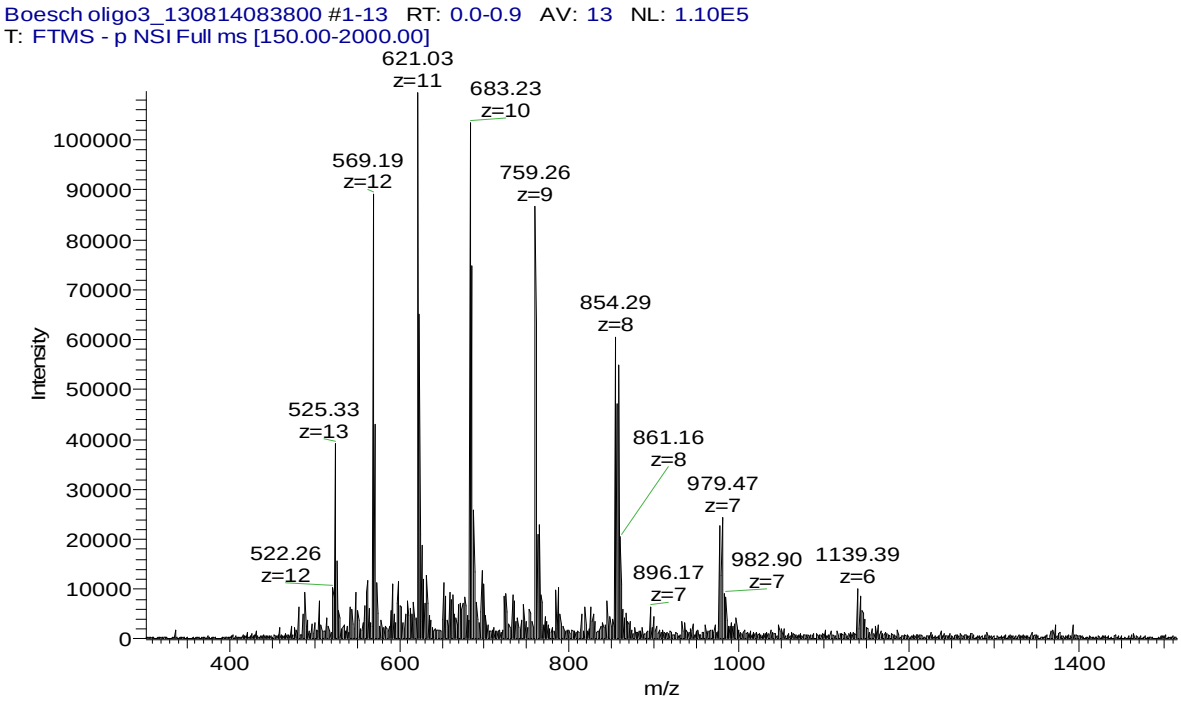


**Figure S11.** HRMS spectrum of oligonucleotide **8**.

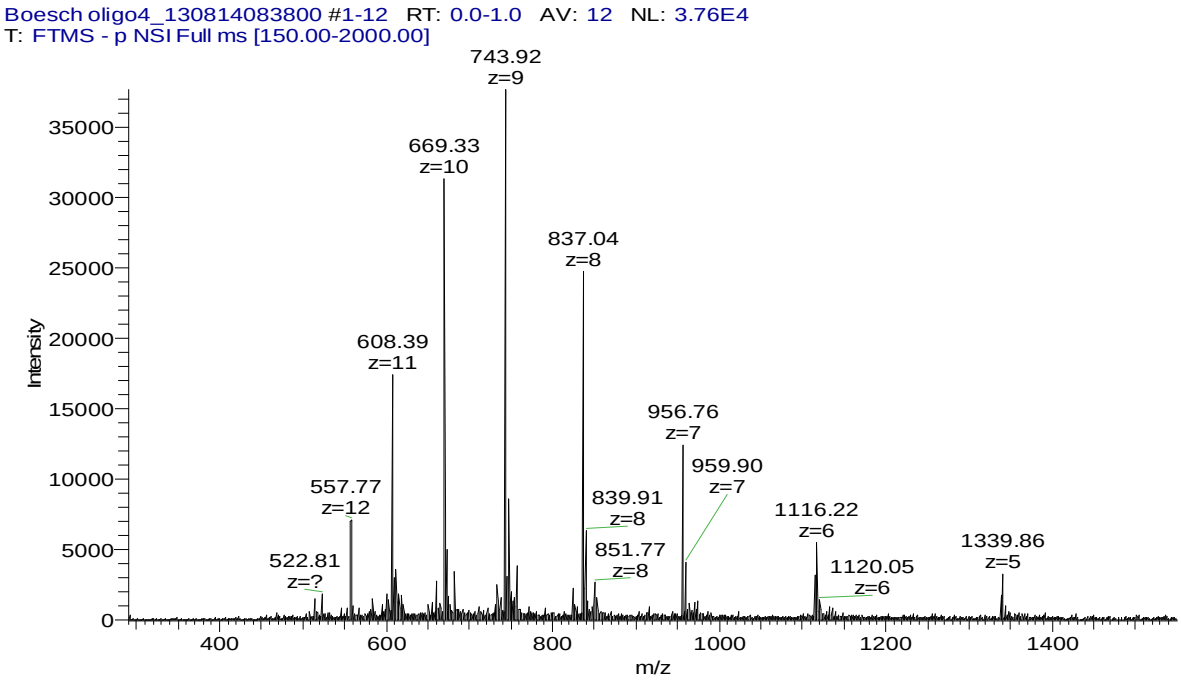


**Figure S12.** HRMS spectrum of oligonucleotide **9**.

**5. UV-vis melting curves.**

Thermal melting experiments were carried out using a block temperature controller, and data were collected with Varian WinUV software at 260 and 370 nm (cooling-ramp in the temperature range of 20-90 °C, temperature gradient of 0.5 °C/min).

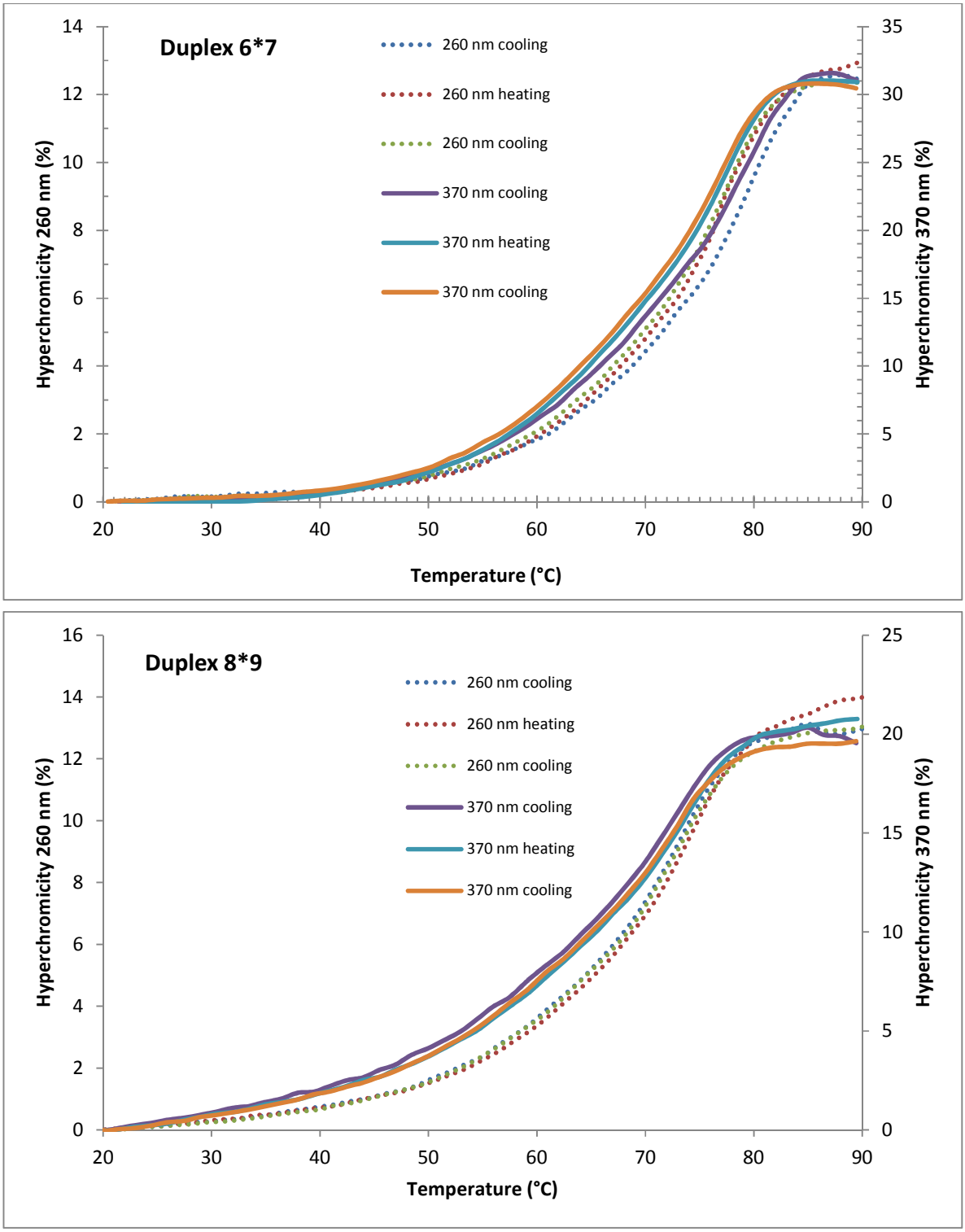


**Figure S13.** UV-vis melting curves of duplexes. Conditions: 10 mM sodium phosphate buffer pH 7.0, 0.1 M NaCl, oligonucleotides 1.0 μM each strand.

**6. Temperature-dependent CD spectrum of duplex 8*9.**

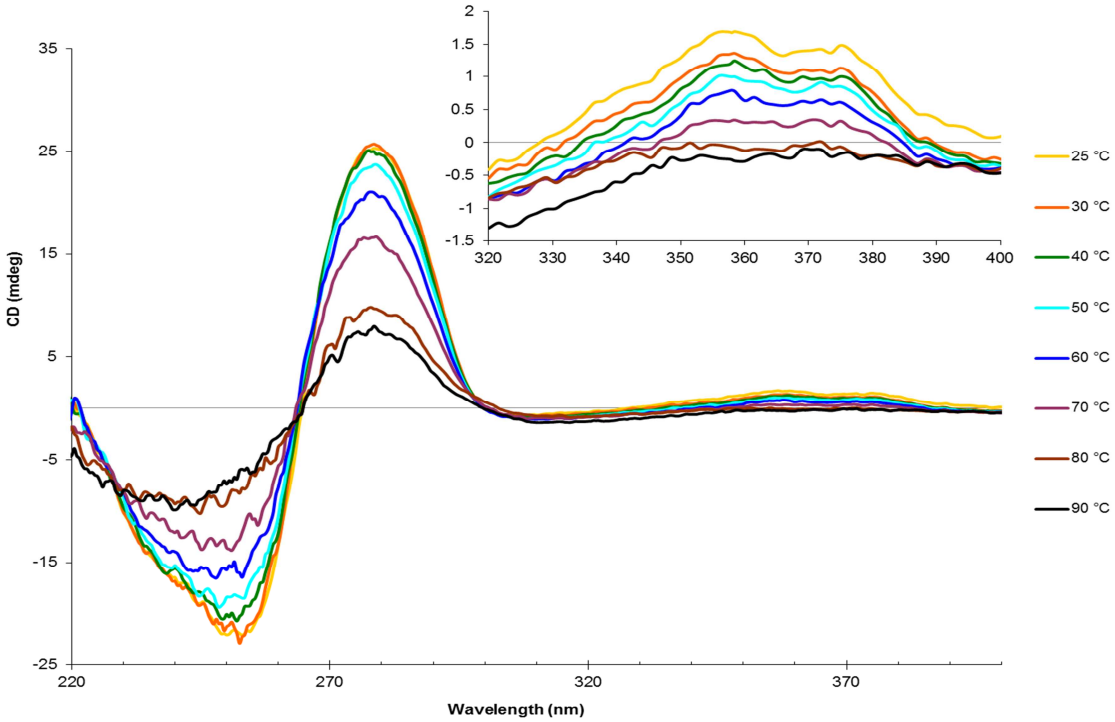


**Figure S14**. Temperature dependent CD spectrum of duplex **8*9**. Oligo conc. 5.0 µM each strand.

**7. References**

(1) Berlman I.B., *Handbook of Fluorescence Spectra of Aromatic Molecules*, 2nd ed. Academic Press, New York and London 1971

(2) S.Fery-Forgues and D. Lavabre, *J. Chem. Educ.*, 1999, **76**, 1260