SUPPORTING INFORMATION

Surface-modified ZnSe Waveguides for Label-free Infrared Attenuated Total Reflection Detection of DNA Hybridization

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Figure S1 displays the chemical modification of the ZnSe surface for determining the DNA hybridization event via IR-ATR spectroscopy. An acid-terminated surface (Fig. S1a) was chemically activated with NHS/EDC (Fig. S1b) for 1h at room temperature. This resulted in an appearance of new peaks in the IR-ATR spectrum (1815, 1787, and 1739 cm^{-1}), which are assigned to the succinimidyl ester (i.e., the stretching modes of the carbonyl functionality at 1815 and 1787 cm^{-1} are characteristic of the succinimidyl moiety).

After exposition of the substrate to the probe DNA and blocking using ethanolamine, the IR-ATR spectrum of the DNA-modified surface (Fig. S1c) reveals the disappearance of all three modes resulting from the NHS ester groups, and the appearance of peaks at 1650 and 1550 cm^{-1}, which are assigned to the carbonyl function and the CNH vibration of the amide. The phosphate and glycoside groups of the DNA backbone are evident at 1550, 1292, and 1100 cm^{-1}. After DNA hybridization (Fig. S1d), an increase of the bands assigned to DNA is evident.

Furthermore, a shift from 1100 cm^{-1} to 1064 cm^{-1} was observed suggesting that these bands permit the distinction between ssDNA and dsDNA, thereby enabling the direct and label-free detection of DNA hybridization at ZnSe surfaces via IR-ATR spectroscopy.

In addition, control experiments (Figure S2) were performed with a 5bp-mismatched DNA sequence (5'-AT**T** TC**T** **G**GG **T**AT TGA G**C**G-3', 20 μM mol), and did not reveal signatures indicating unspecific binding. As no shift from 1100 cm^{-1} to 1064 cm^{-1} was observed during this control experiment, further evidence for the utility of this shift in identifying hybridization events with the target DNA is provided (Fig. S1d).

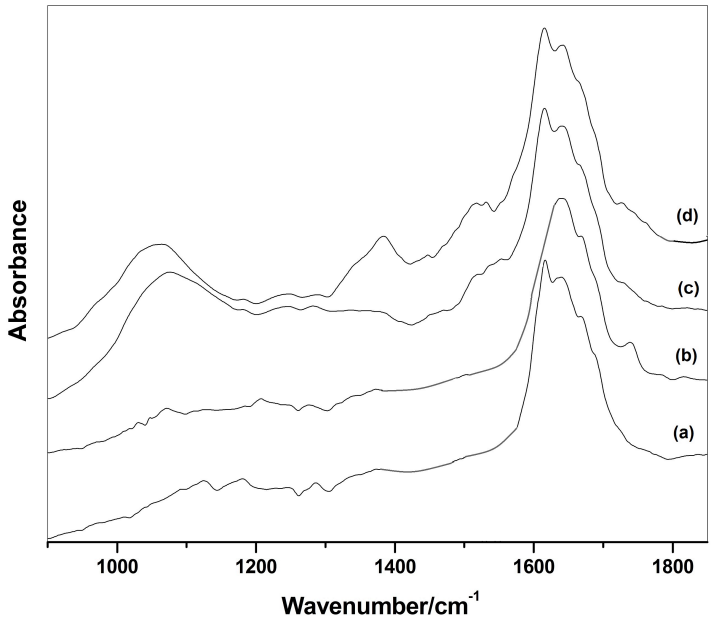

Figure S1. IR-ATR spectra of the ZnSe surface modified with undecylenic acid (a), after the surface was reacted with NHS/EDC for 1 h at room temperature (b), after exposure to probe DNA and blocking using ethanolamine (c), and after DNA hybridization (d). The IR spectra shown here are not baseline corrected.

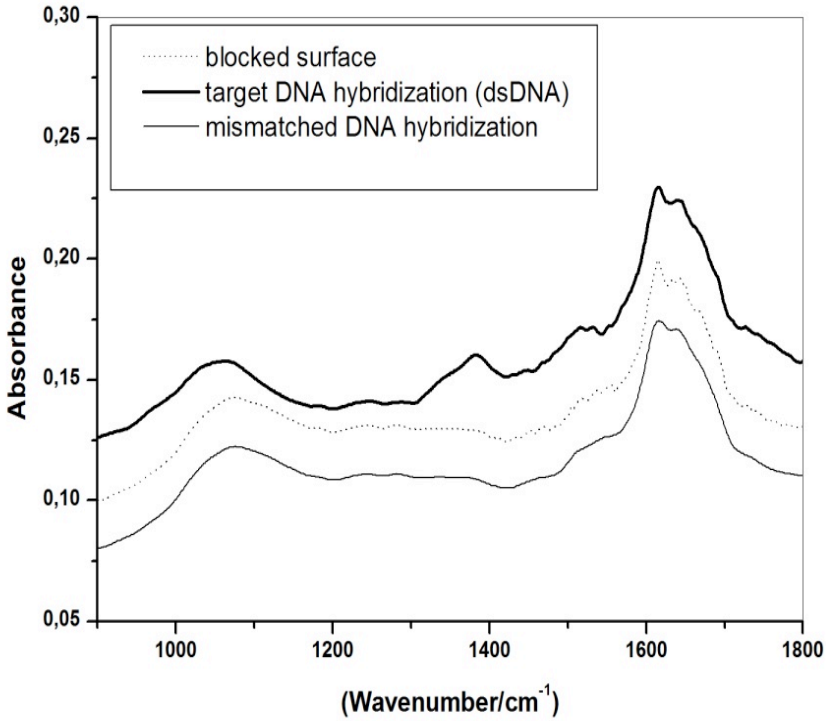

Figure S2. IR-ATR spectra of the DNA-modified waveguide surface after the blocking step, after exposure to 5bp-mismatched DNA, and after hybridization with the target DNA sequence. The IR spectra shown here are not baseline corrected.