Supplementary Material (ESI) for Chemical Communications
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Supplementary information

Sugar-thioacetamide Backbone in Oligodeoxyribonucleosides for Specific Recognition of Nucleic Acids
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Table of contents

S2: General experimental procedure, spectral data of compounds 6 and 14.
(S3-S6): MALDI-TOF and LCMS Mass spectra of compounds 6 and 14.
(S7-S12): HPLC profiles of TANA 15, TANA 16, TANA 17, TANA 18, and TANA 19, aegPNA20.
(S13-S18): Mass spectra (MALDI-TOF) of TANA 15, TANA 16, TANA 17, TANA 18, TANA 19, aegPNA20.
(S19): Melting curves of TANA 17, TANA 18, TANA 19, aegPNA20 with RNA22 and their corresponding derivatives.
(S20): Melting curves of TANA 15 and TANA 16 with RNA22 and 23 and corresponding derivative curves.
(S21): UV-Job’s plot for TANA 15:RNA22
**General Experimental Procedure**: Melting points of samples were determined in open capillary tubes and are uncorrected. IR spectra were recorded on an infrared Fourier Transform spectrophotometer using Chloroform, Nujol and KBr pellets. Column chromatographic separations were performed using silica gel 60-120 mesh, and 230-400 mesh, solvent systems EtOAc/Pet ether and pure MeOH/DCM. $^1$H and $^{13}$C were obtained using Bruker AC-200 (200 MHz) and 500 MHz NMR spectrometers. The chemical shifts are reported in delta (δ) values. The optical rotations were recorded in an ADP220 Polarimeter. Mass spectra were obtained either by LCMS and MALDI-TOF mass spectrometry techniques. Oligomers were purified and analyzed by RP HPLC, C18 column and MALDI-TOF mass spectrometry.

**3’-[9-fluorenylmethoxycarbonyloxy]-amino-3’-deoxy thymidin -5’-thioacetic acid, 6.**

M.p.147-150 °C. $[\alpha]_D^{20} +16^\circ$ (c 0.5;CH$_3$OH). IR, ν(cm$^{-1}$), (Chloroform) 3236.98, 2927.74, 2358.78, 1704.96, 1677.95, 1529.45, 1463.87. $^1$HNMR:(DMSO-d$_6$,200MHz) δ 1.78(s,3H;5-CH$_3$), 2.06-2.28(m,2H;2,2’’-H), 3.15-3.38(m,6H; 4'-H,3'-H,5',5''-H,-CH$_2$ Fmoc), 3.72-3.96(t,1H;1'-H), 7.27-7.96(m,10H;Fmoc-H). $^{13}$C(DMSO-d$_6$,200MHz) δ 12.63(CH$_3$), 34.68(CH$_2$), 47.28(CH), 53.75(CH), 62.66(CH$_2$), 83.25(CH), 110.57(C), 120.67(CH), 125.64(CH), 127.68(CH), 130.76(CH), 136.76(CH), 141.31(C), 144.29(C), 150.94(C=O), 156.44(C=O), 164.48(C=O), 172.04(C=O). Anal Calcd (%) forC$_{27}$H$_{27}$N$_3$O$_7$S: C 60.19; H 5.246; N 7.805; S 5.955; Found C 60.79; H 5.02; N 7.46; S 6.03. MS, M+Na$,^+$ Calculated 560.33; Observed, MALDI-TOF 560.38, LCMS 560.06.

**3’-[9-fluorenylmethoxycarbonyloxy]-amino-3’-deoxy 5-methyl cytidine 5’-thioacetic acid, 14**

M.p.160-163°C. $[\alpha]_D^{20} +18^\circ$ (c 0.5;CH$_3$OH).

IR, ν(cm$^{-1}$), (nujol) 3283.26, 2923.88, 2854.45, 1714.6, 1666.38 (cm$^{-1}$). $^1$HNMR: (CDCl$_3$+CD$_3$OD,200MHz) 2.26-2.55(m,2H;2,2’’-H), 3.22-3.44(m,2H;SCH$_2$), 3.7-4.39(m,4H;4'-H,5',5''-H,3’-H), 6.09(s,1H;1'-H), 7.29-8.07(m,10H;6-H,Fmoc-H). $^{13}$C(DMSO-d$_6$) 13.4(CH$_3$), 34.07(CH$_2$), 73.32-73.38(CH), 80.16(CH), 110.71(C), 120.74(CH), 125.69(CH), 127.97(CH), 130.76(CH), 136.76(CH), 141.31(C), 144.29(C), 150.94(C=O), 156.44(C=O), 164.48(C=O), 172.04(C=O). Anal Calcd (%) forC$_{27}$H$_{27}$N$_3$O$_7$S: C 60.19; H 5.246; N 7.805; Found C 60.79; H 5.02; N 7.46; S 6.03. MS, M+Na$,^+$ Calculated 536.60, 559.39; Observed MALDI-TOF, 559.43; LCMS 537.06.
MALDI-TOF mass of compound 6
LCMS of compound 6
MALDI-TOF of compound 14
LCMS of compound 14
HPLC profile of **TANA15**

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<th>Result (%)</th>
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HPLC profile of TANA16

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Data File: c:\data\data\pQA\k6Xrun
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Sample ID: K6
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Injection Method: c:\star\method1.mth
Run Time (min): 20.002
Workstation: Varian Star #1
Operator (Calc): SSK/MVM
Calc Date: 12/23/05 04:18:37 PM
Times Calculated: 1
Calculation Method: c:\star\method1.mth
Verification Method: Varian Star #1
Instrument (Calc): Analysis
Calculation Type: Percent
Calibration Level: N/A
HPLC profile of **TANA17**

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**Graph:**
- **mV:**
  - 0 to 150
- **Minutes:**
  - 0 to 15

**Table:**
- **Peak No:** 1, 2, 3
- **Ret. Time (min):** 1.911, 2.427, 10.046
- **Width 1/2 (sec):** 12.3, 0.0, 6.6
- **Peak Area (counts):** 15652, 9796, 136043
- **Result (i):** 1.1294, 0.7069, 98.1628
HPLC profile of **TANA18**

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- **Calculation Method:** c:star/method 1.mth
- **Instrument (Calc):** Varian Star #1
- **Run Mode:** Analysis
- **Peak Measurement:** Percent
- **Calibration Level:** N/A
- **Verification Tolerance:** N/A

**Graph:**
- X-axis: Minutes
- Y-axis: mV
- Peak at approximately 2.5 minutes with peak area counts of 12115 and result of 0.3805.
HPLC profile of **TANA19**

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HPLC profile of aeg PNA 20

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MALDI-TOF mass of **TANA15**
MALDI-TOF mass of TANA16
MALDI-TOF of TANA17
MALDI-TOF mass of TANA18
MALDI-TOF mass of TANA19
MALDI-TOF mass of aeg PNA 20
**UV-Tm measurements:** The complementary DNA and RNA oligomers were synthesized on an Applied Biosystems DNA Synthesizer. The concentration was calculated on the basis of absorbance from the molar extinction coefficients of the corresponding nucleobases. The complexes were prepared in 10 mM sodium phosphate buffer, pH 7.4 containing NaCl (10 mM) and were annealed by keeping the samples at 90°C for 5 minutes followed by slow cooling to room temperature. Absorbance versus temperature profiles were obtained by monitoring at 260 nm with Perkin-Elmer Lambda 35 spectrophotometer scanning from 10 to 85°C at a ramp rate of 0.2/0.5°C per minute. The data were processed using Microcal Origin 6.0 and Tm values derived from the derivative curves.

Fig A. Melting curve of TANA 17, 18, 19 & aegPNA20 with RNA 22 B. Corresponding derivative curve.
Fig: C. Melting curve of TANA15 and TANA16 with RNA22 and RNA23, 10mM phosphate buffer (pH=5.5) and 10 mM NaCl concentration. B. Corresponding derivative curve.

Fig: E UV-melting curve of TANA 15 & 16, DNA 24 with complementary RNA 22 and RNA 23 F. Corresponding derivative curves.
Fig: G UV-Jobs Plot of TANA15 with RNA22