## Synthesis of "clickable" m<sub>3</sub>G-CAP analogues.

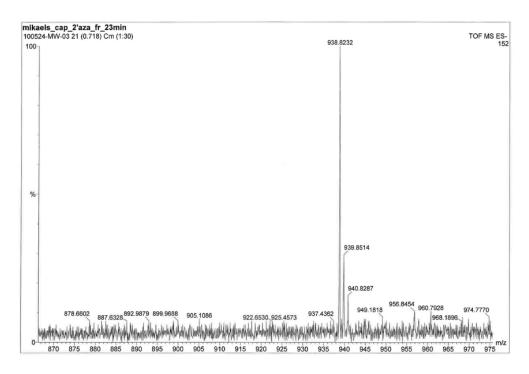
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## **Supplementary information**

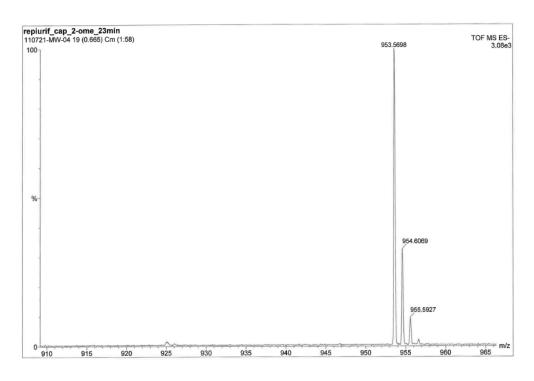
- 1. Mass spectra of m<sub>3</sub>G-CAP constructs 1-4.
- 2. HPLC Chromatograms showing examples of crude reaction mixtures after capping of clickable mono and trinucleotides.
- 3. HPLC Chromatogram showing crude oligonucleotide (ON)-PATA conjugate.
- 4. Mass spectra of ON-PATA conjugate.
- 5. Additional HPLC Chromatograms showing examples of crude reaction mixtures after conjugation of the 18merRNA with the clickable m<sub>3</sub>G-CAP's.
- 6. Mass spectra of 18merRNA-m<sub>3</sub>G-CAP1-4 ON conjugates.
- 7. Mass spectra of 5'-phosphate-AUA(5)-ON conjugate.
- 8. Mass spectra of compounds 20 and 21.

### 1. Mass spectra of m<sub>3</sub>G-CAP analogues 1-4.

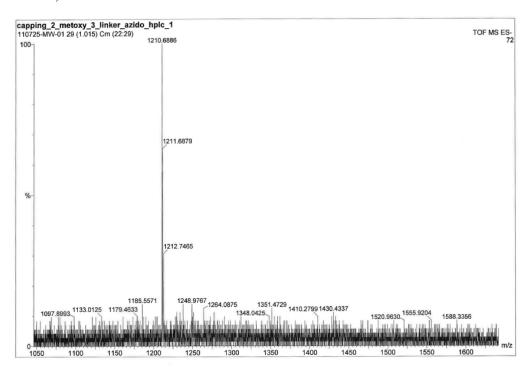
**m<sub>3</sub>G-CAP analogue 1**: (MS(ES<sup>-</sup>TOF) m/z) [M]<sup>-1</sup> m/z calculated: 939.17, found: 938.82;



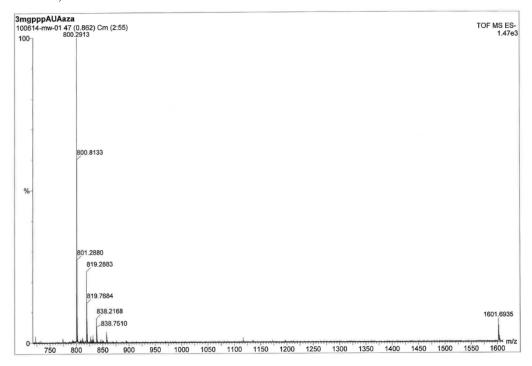
 $m_3G$ -CAP analogue 2: (MS(ES TOF) m/z) [M]<sup>-1</sup> m/z calculated: 953.19, found: 953.56;



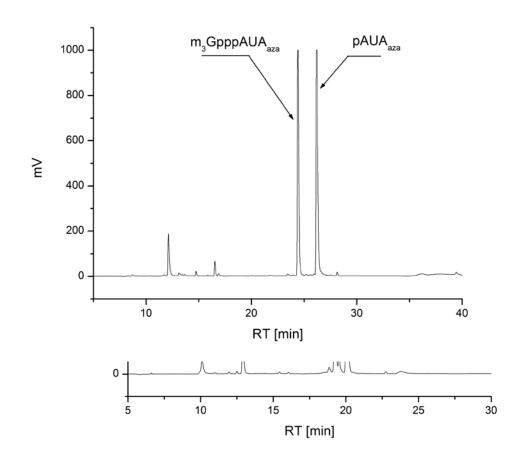
**m<sub>3</sub>G-CAP analogue 3**: (MS(ES<sup>-</sup>TOF) m/z) [M]<sup>-1</sup> m/z calculated: 1210.27, found: 1210.68;



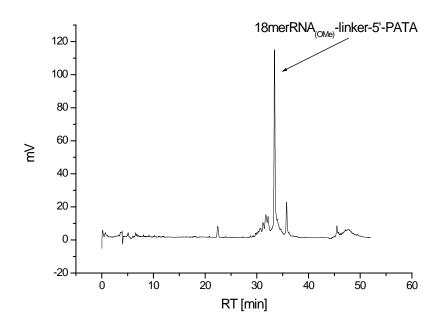
**m<sub>3</sub>G-CAP analogue 4**: (MS(ES<sup>-</sup>TOF) m/z) [M]<sup>-1</sup> m/z calculated: 1602,28 found: 1601.69;



- 2. HPLC Chromatograms showing examples of crude reaction mixtures after capping of clickable mono and trinucleotides.
- a) HPLC chromatogram of crude reaction mixture in synthesis of m3G-Cap construct 3.
- a) HPLC chromatogram of crude reaction mixture in synthesis of m3G-Cap construct 4.

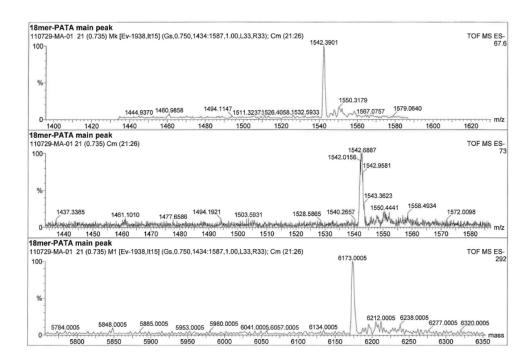


# **3. HPLC Chromatogram showing crude ON-PATA conjugate** (after removal from solid support with methanolic ammonia).



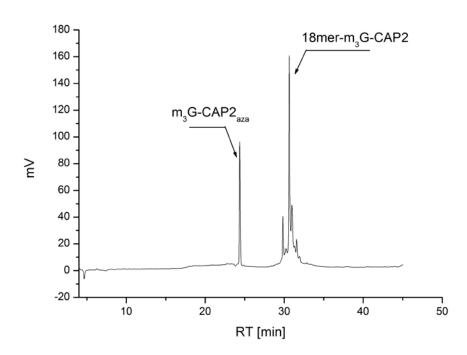
**4. Mass spectra of ON-PATA conjugate.** Molecular weights of the conjugates were reconstructed from the m/z values of the multiply charged ions using the mass deconvolution program (MAXENT)

ES-MS, calculated (M) 6175, found 6173

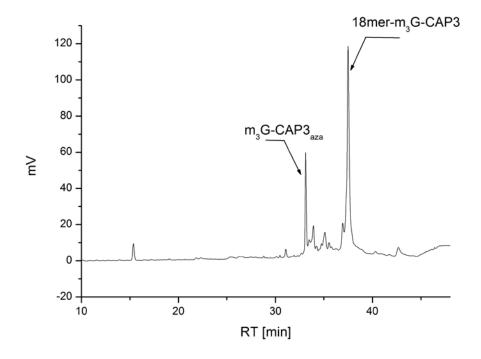


# 5. HPLC Chromatograms showing examples of crude reaction mixtures after conjugation of the 18merRNA with the clickable $m_3G\text{-}CAP$ 's.

### a) HPLC Chromatogram of crude 18merRNA-CAP2

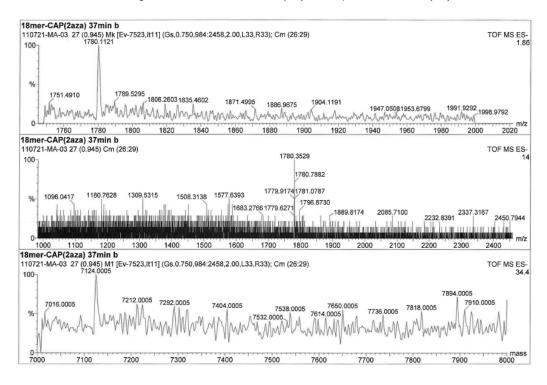


## b) HPLC Chromatogram of crude 18merRNA-CAP3

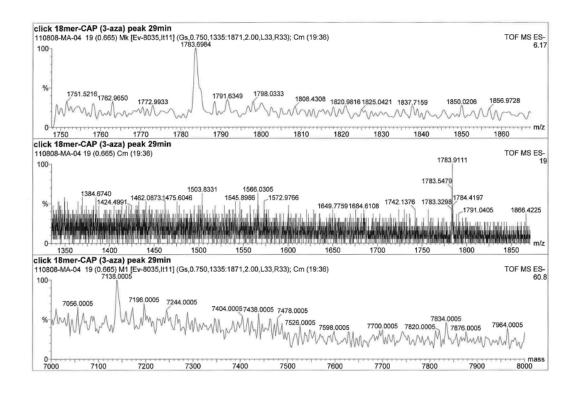


#### 6. Mass spectra of m<sub>3</sub>G-CAP(1-4)-ON conjugates.

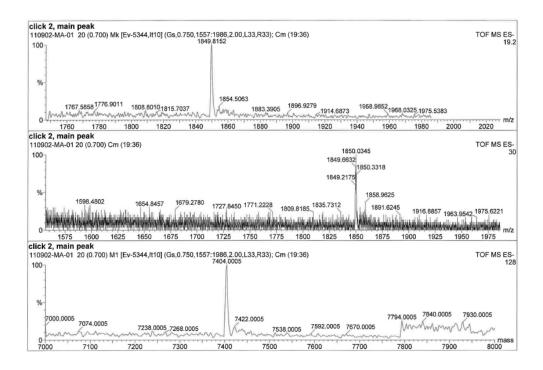
#### **18mer-m<sub>3</sub>G-CAP1**: calculated (M) 7120, found 7124 (M).



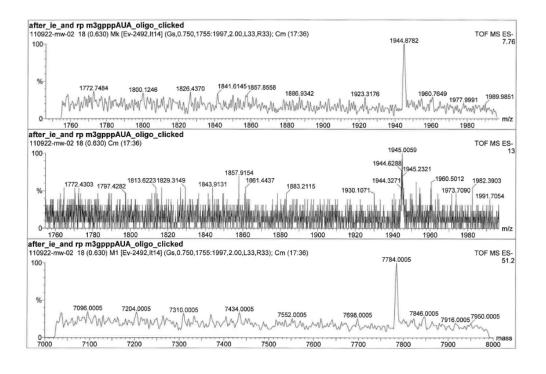
**18mer-m<sub>3</sub>G-CAP2**: calculated (M) 7134, found 7138 (M),



#### **18mer-m**<sub>3</sub>**G-CAP3**: calculated (M) 7405, found 7404 (M),

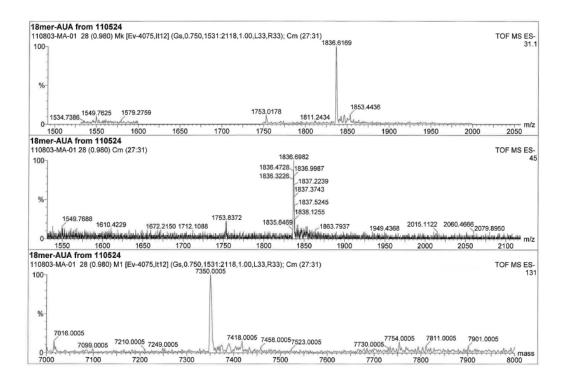


#### **18mer-m<sub>3</sub>G-CAP4**: calculated (M) 7783, found 7784 (M).



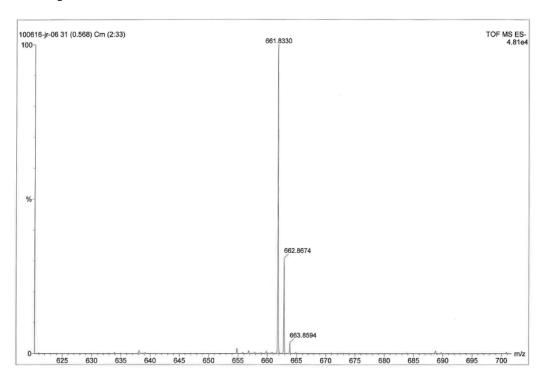
## 7. Mass spectra of 5'-phosphate-AUA(5)-ON conjugate.

ES-MS, calculated (M) 7315, found 7350 (M+K).



## 8. Mass spectra of compounds 20 and 21.

Compound 20: m/z calculated for [M-]: 662.23, observed mass: 661.83



**Compound 21:** *m/z* calculated for [M-]: 742.20, found: 742.03

