

# Highly improved ESI-MS detection of G-quadruplex-folded oligonucleotides and their complexes with small molecules

M. Scalabrin,<sup>§</sup> M. Palumbo<sup>‡</sup> and S. N. Richter<sup>§\*</sup>

<sup>§</sup> *Department of Molecular Medicine, University of Padua, via Gabelli 63, 35121 Padua, Italy*

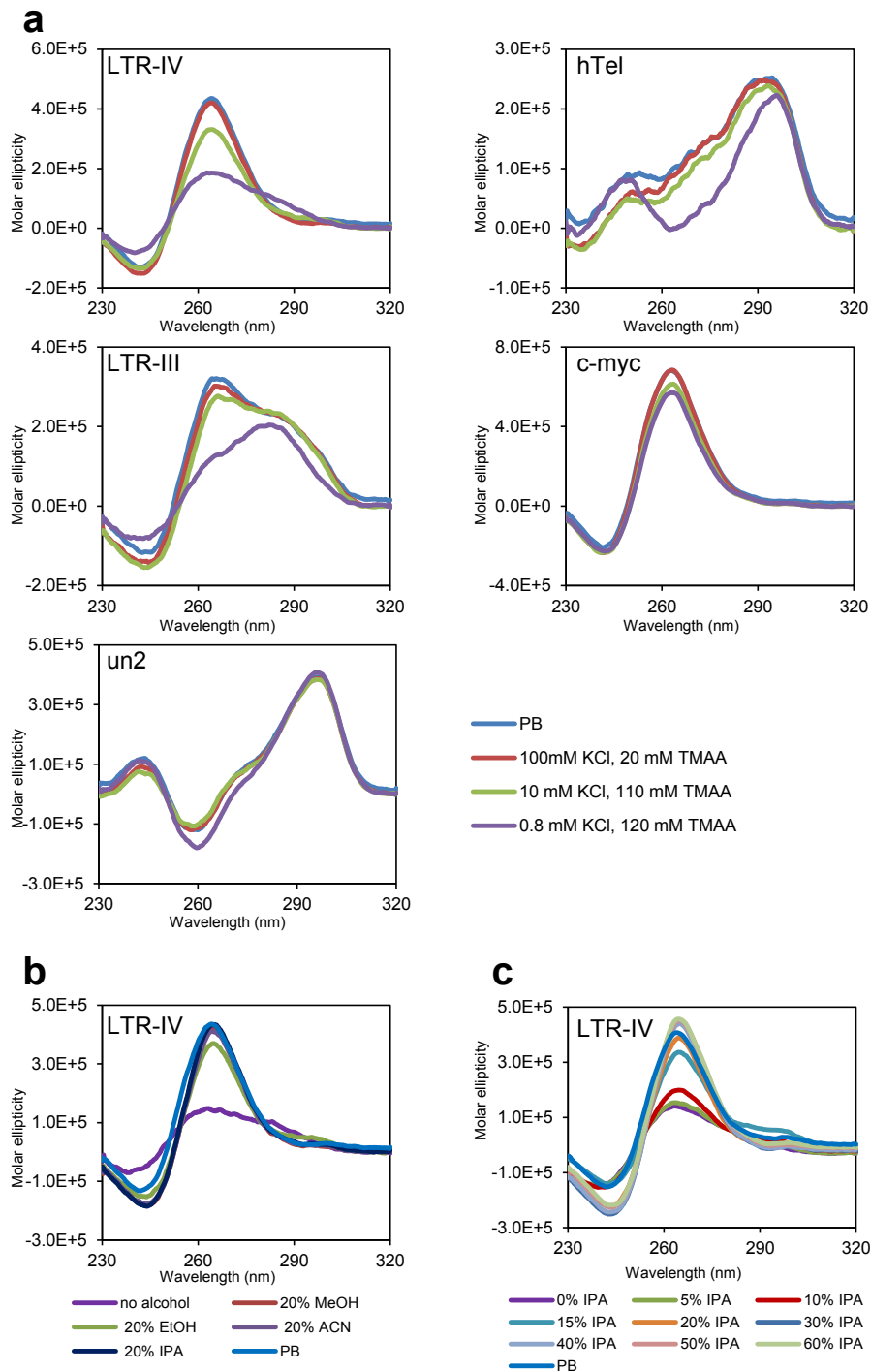
<sup>‡</sup> *Department of Pharmaceutical and Pharmacological Sciences, University of Padua, via Marzolo 5, 35131 Padua, Italy.*

## Table of Contents

<b>Table S1.</b> Oligonucleotides used in this study.	pag. 2
<b>Figure S1.</b> Dichroic spectra of the tested G4 forming oligonucleotides	pag. 3
<b>Figure S2.</b> ESI-MS full spectra of the zoomed in spectra shown in Fig 1b.	pag. 4
<b>Figure S3.</b> ESI-MS full spectra of the zoomed in spectra shown in Fig 2.	pag. 9
<b>Figure S4.</b> ESI-MS spectra of decreasing amounts of LTR-IV with B19	pag. 10

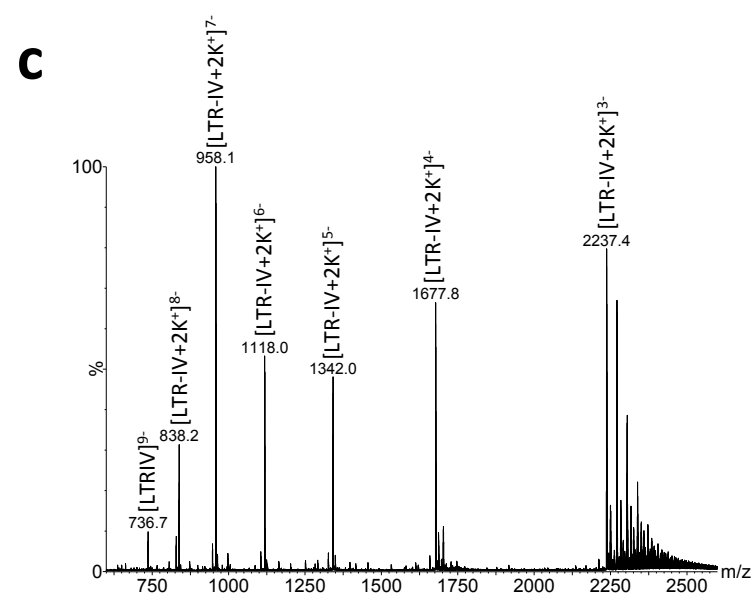
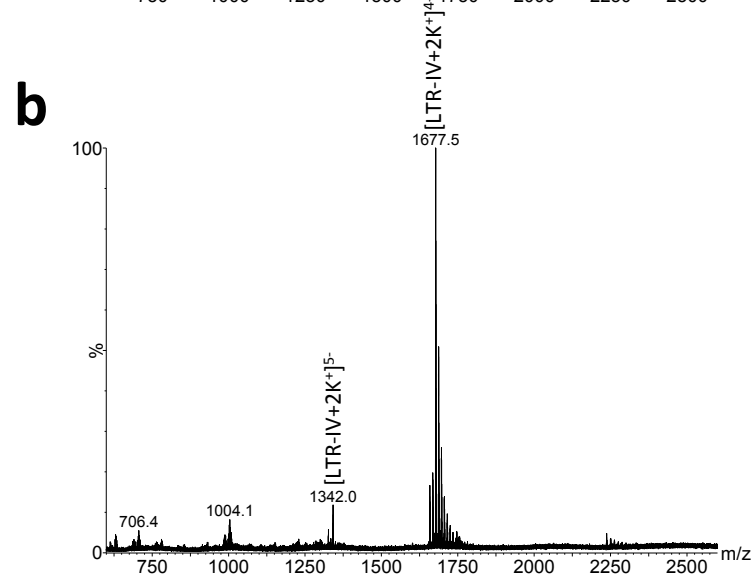
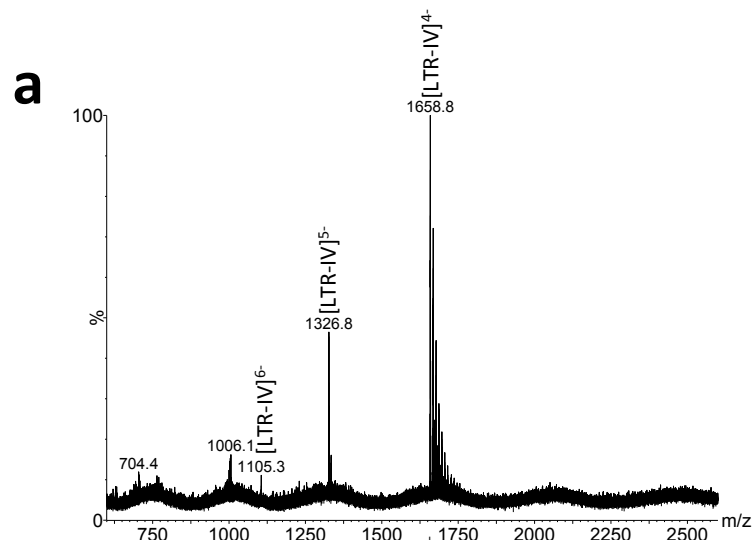
**Table S1.** Oligonucleotides used in this study.

<b>Name</b>	<b>Sequence 5'-3'</b>
LTR-IV	d(TGGGCGGGACTGGGGAGTGGT)
LTR-III	d(TGGGAGGCCTGGCCTGGGCGGGACTGGGGT)
un2	d(GGGGGCGAGGGGCGGGAGGGGGCGAGGGG)
hTel	d(AGGGTTAGGGTTAGGGTTAGGG)
c-myc	d(TGGGGAGGGTGGGGAGGGTGGGGAAGG)



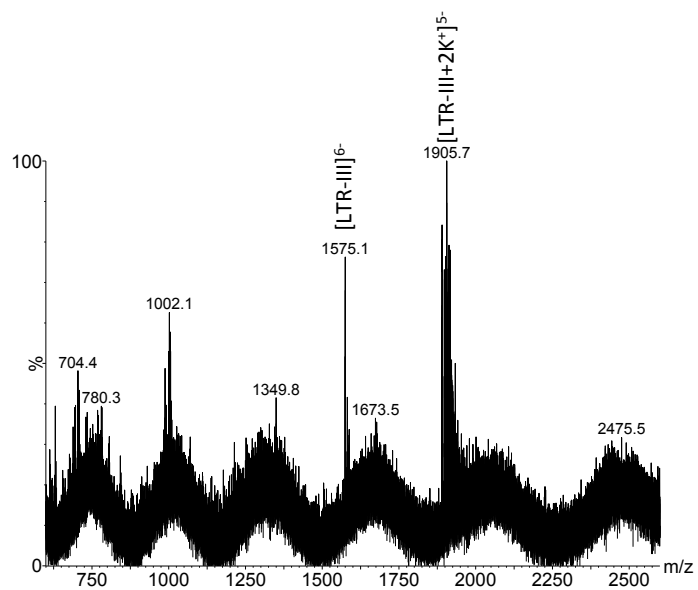
**Figure S1.** Dichroic spectra of the tested G4 forming oligonucleotides. a) CD spectra in 100 mM K<sup>+</sup>, 20 mM K<sub>2</sub>HPO<sub>4</sub>, pH 7.4 (PB) and TMAA buffers, pH 7.4, at different K<sup>+</sup> concentrations. b) CD spectra of LTR-IV in 0.8 mM K<sup>+</sup>, TMAA 120 mM, pH 7.4, in the presence of 20% of the indicated solvents. c) CD spectra of LTR-IV in 0.8 mM K<sup>+</sup>, TMAA 120 mM, pH 7.4, in the presence of the indicated % of IPA. In all panels the reference spectrum was measured in 100 mM K<sup>+</sup>, 20 mM K<sub>2</sub>HPO<sub>4</sub>, pH 7.4 (PB).

# LTR-IV

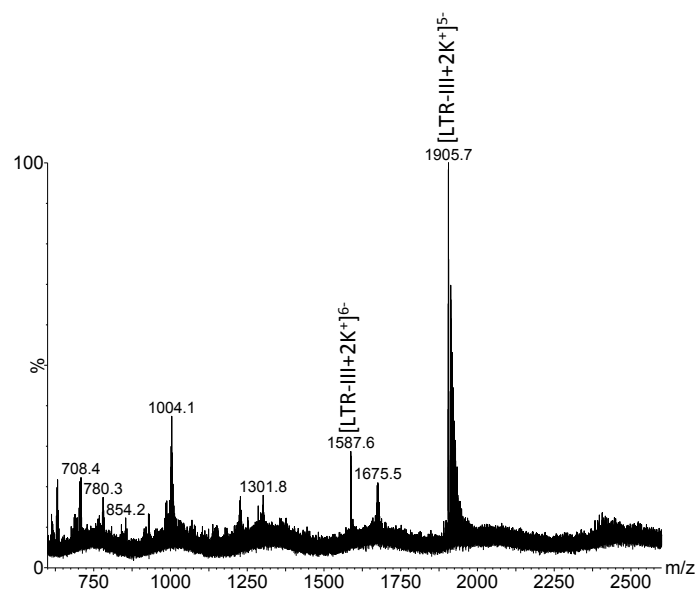


# LTR-III

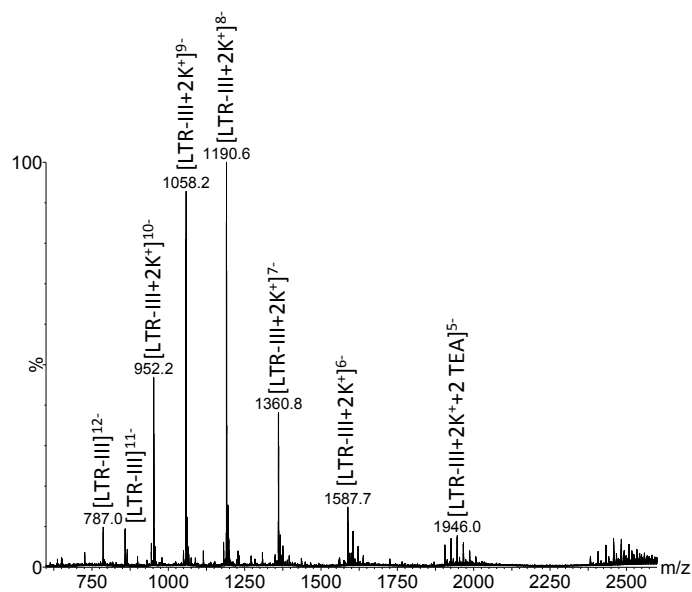
**a**



**b**

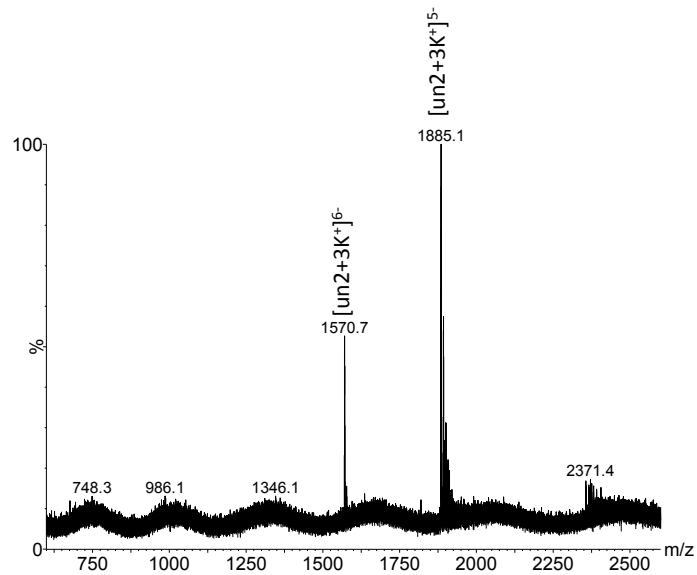


**c**

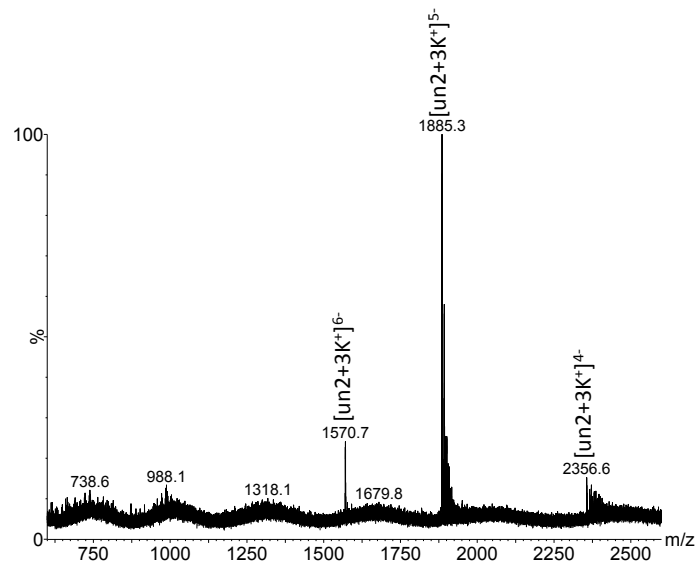


un-2

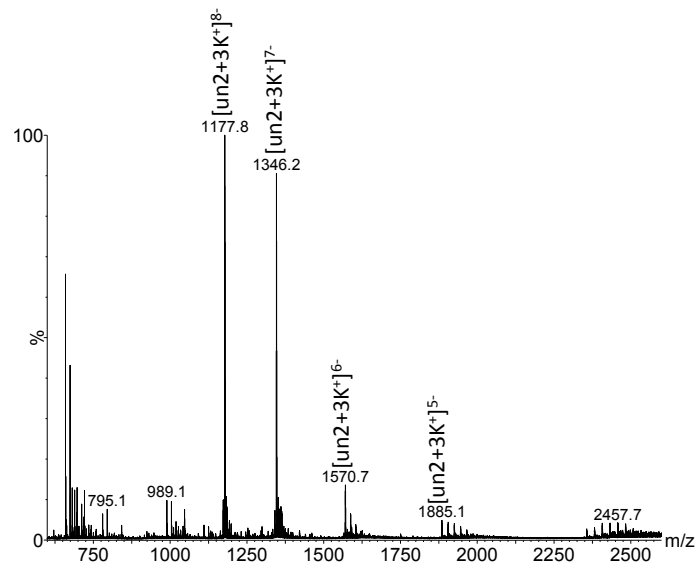
a



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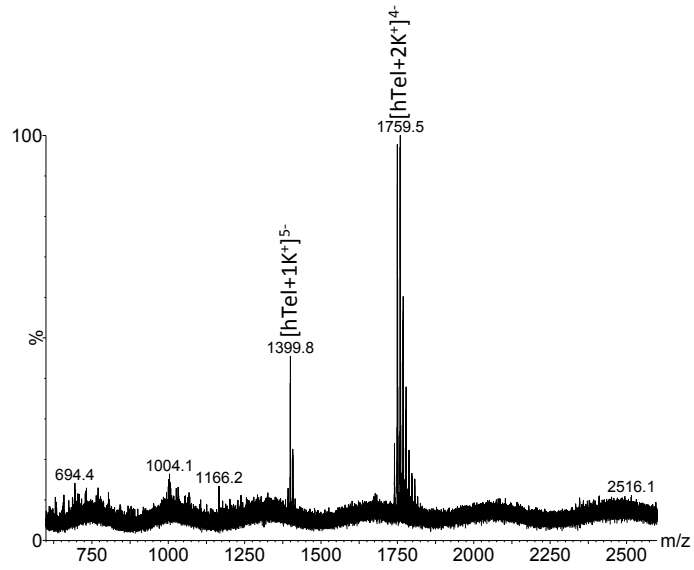


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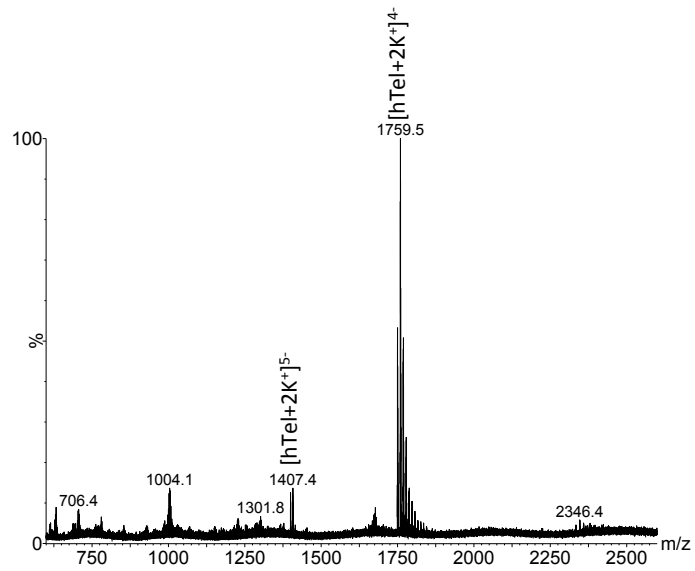


# hTel

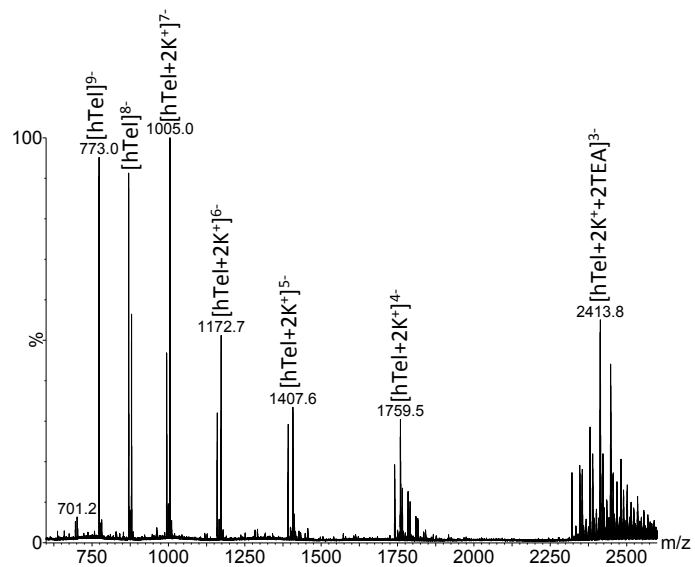
**a**



**b**

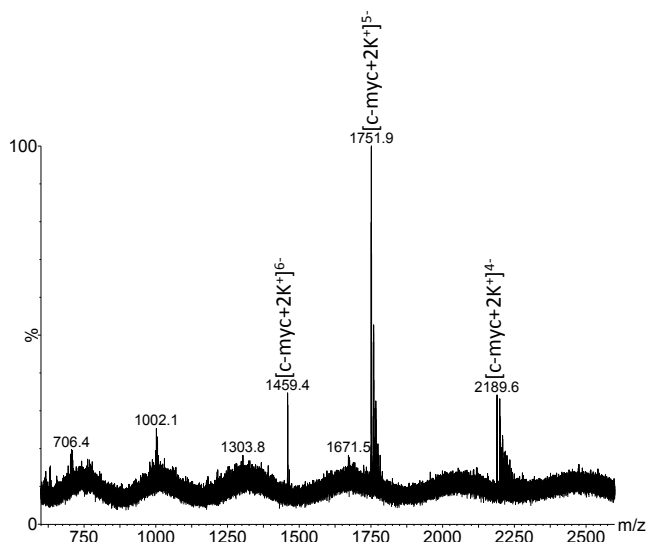


**c**

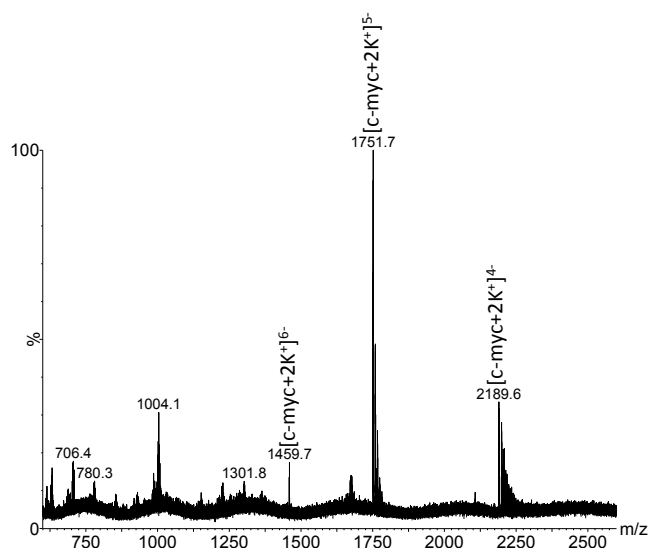


# c-myc

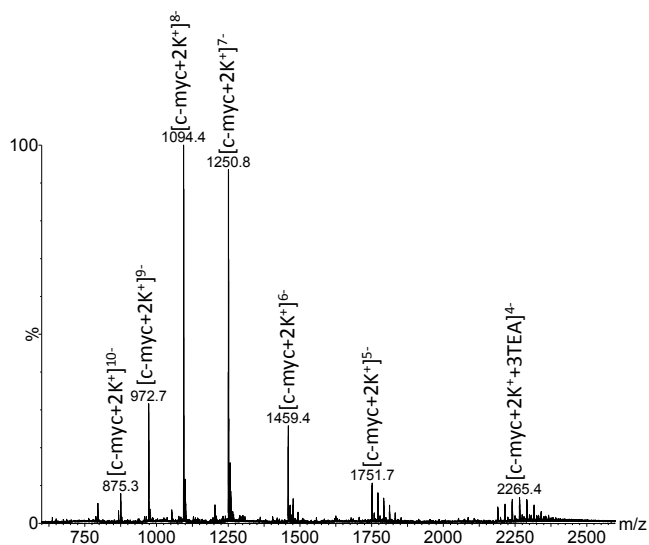
a



b

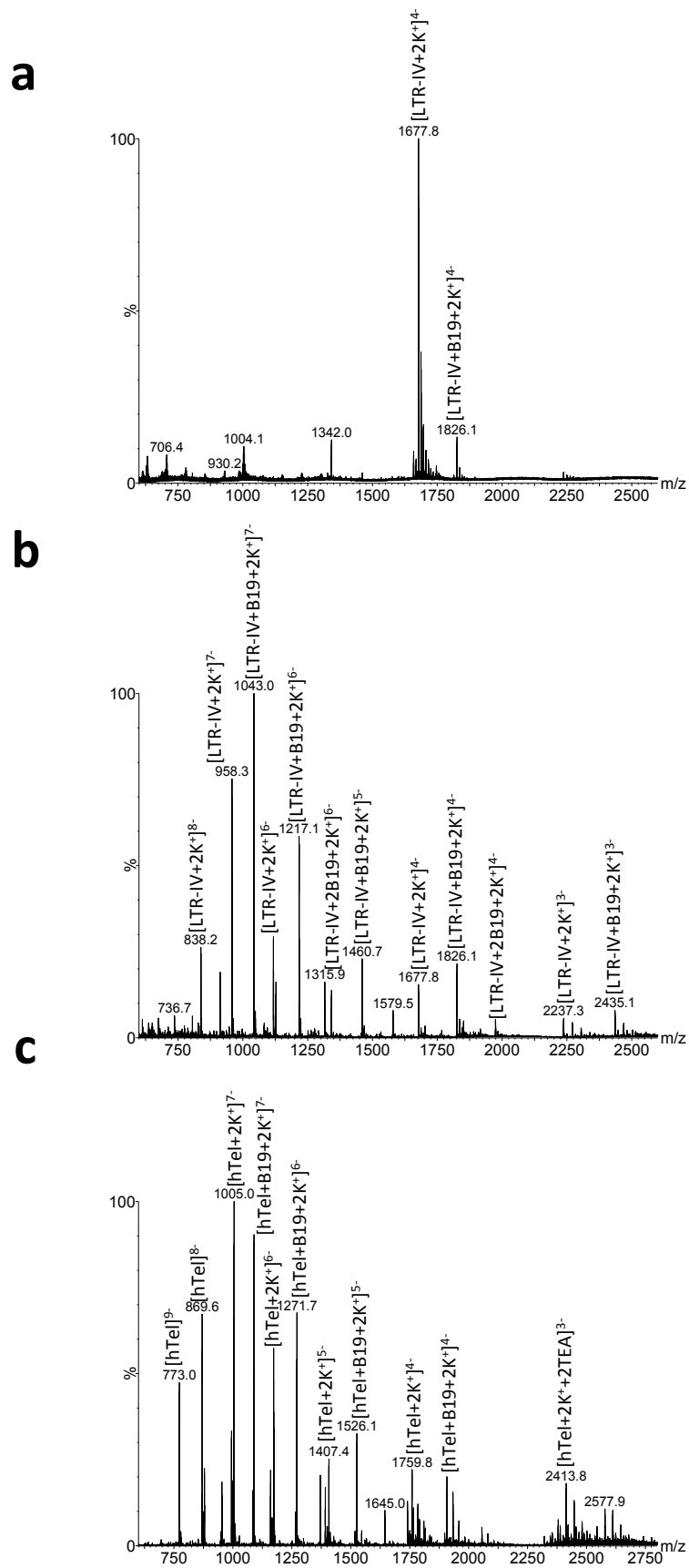


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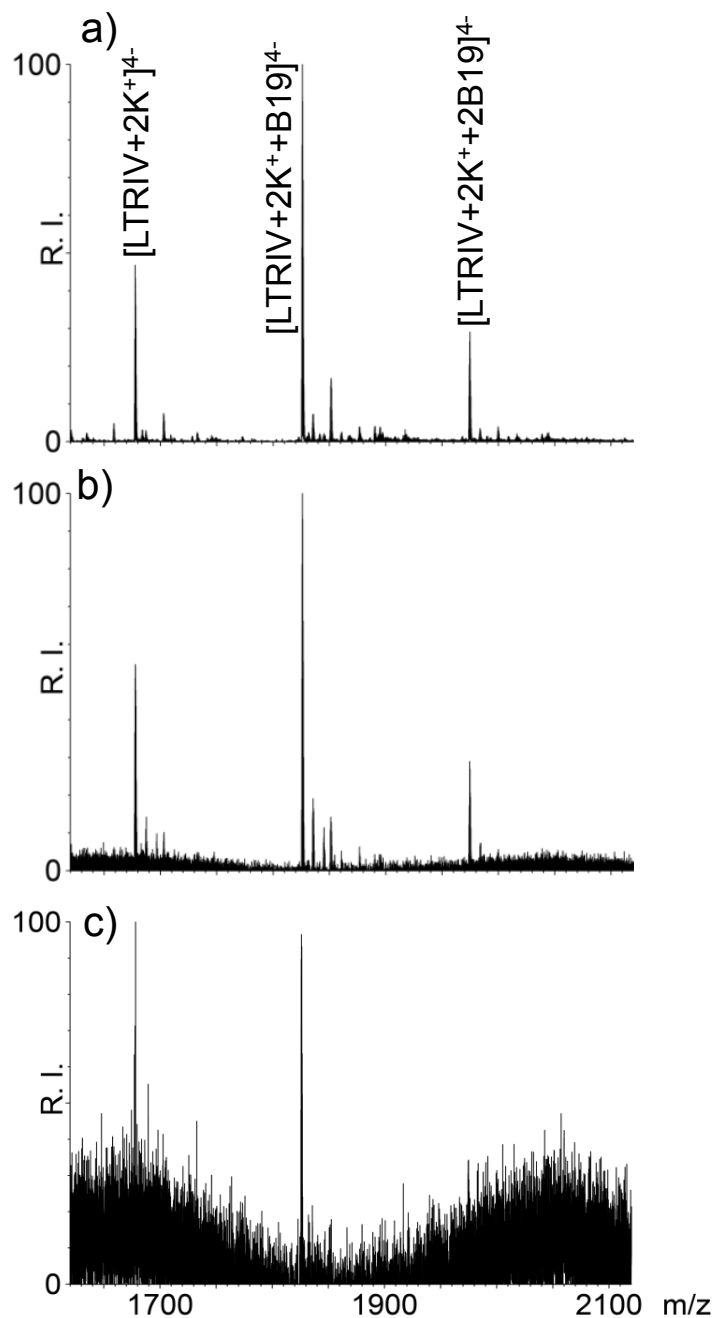
**Figure S2.** ESI-MS full spectra of the indicated oligonucleotides in a) 0.8 mM K<sup>+</sup>, 120 mM TMAA, b) 0.8 mM K<sup>+</sup>, 120 mM TMAA added of 20% IPA, c) 0.8 mM K<sup>+</sup>, TEA/120 mM HFIP added of 20% IPA. These are the full spectra of the zoomed spectra reported in Fig. 1b.





**Figure S3.** ESI-MS full spectra of the zoomed spectra reported in Fig. 2. a) LTR-IV + B19 molar ratio 1:2 in 120 mM TMAA pH 7.4 , 0.8 mM KCl, 20% IPA, b) LTR-IV + B19 molar ratio 1:2 in

TEA/120 mM HFIP pH 7.4 , 0.8 mM KCl, 20% IPA, c) hTel + B19 molar ratio 1:1 in TEA/120 mM HFIP pH 7.4 , 0.8 mM KCl, 20% IPA.



**Figure S4.** ESI-MS spectra of decreasing amounts of LTR-IV with B19. LTR-IV at different concentration, i.e. 4  $\mu\text{M}$  (a) 0.4  $\mu\text{M}$  (b) and 0.04  $\mu\text{M}$  (c) incubated with 2 equivalents of B19 in TEA/HFIP 120 mM pH 7.4, 0.8 mM KCl and 20% IPA.