Supporting Information for:

Replication Past the N^5-Methyl-Formamidopyrimidine Lesion of Deoxyguanosine by DNA Polymerases and an Improved Procedure for Sequence Analysis of In Vitro Bypass Products by Mass Spectrometry.

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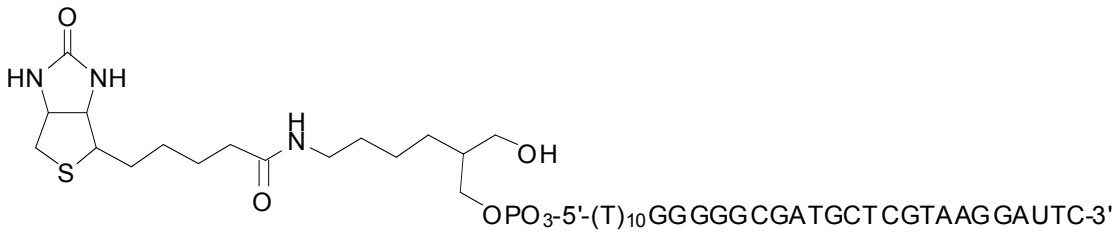

Figure S1. Biotinylated primer.

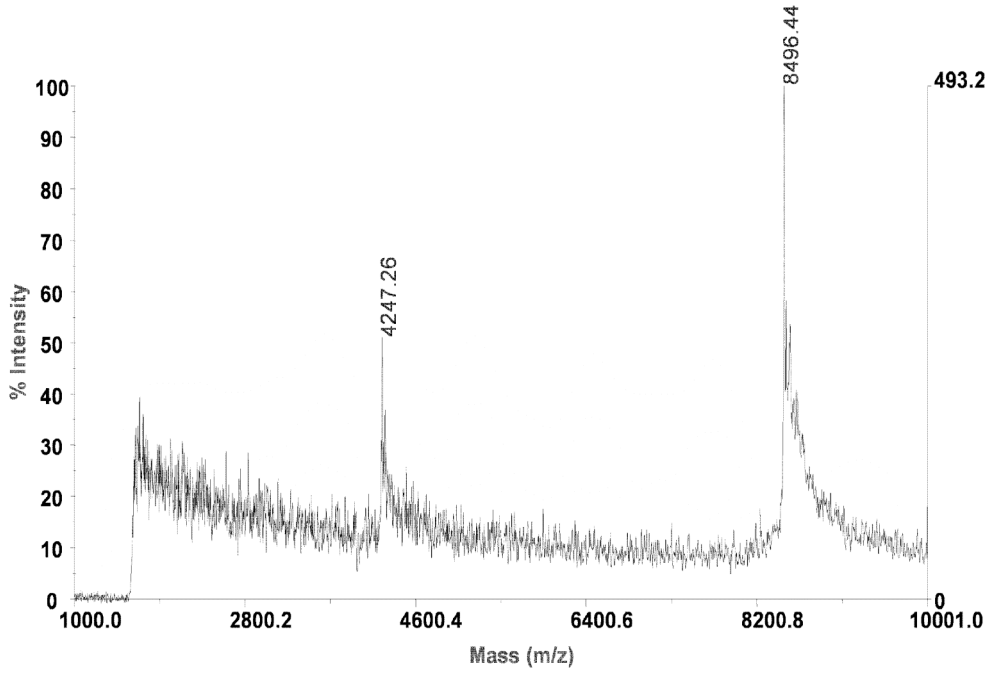

Figure S2. MALDI -TOF spectrum of oligonucleotide **1**.

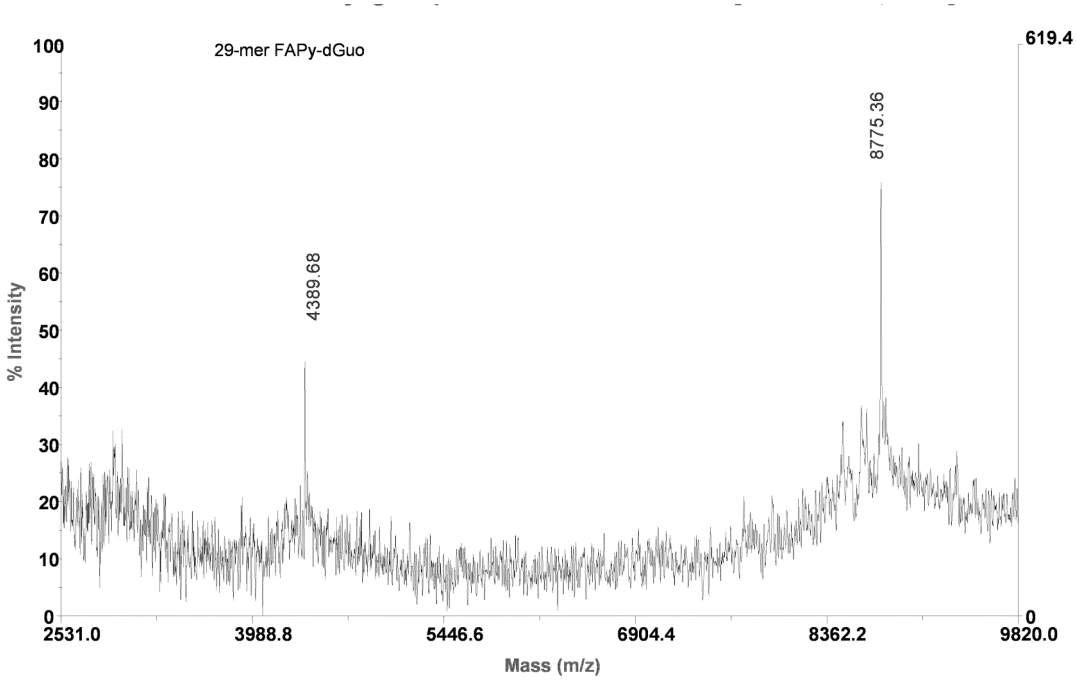

Figure S3. MALDI -TOF spectrum of oligonucleotide **2**.

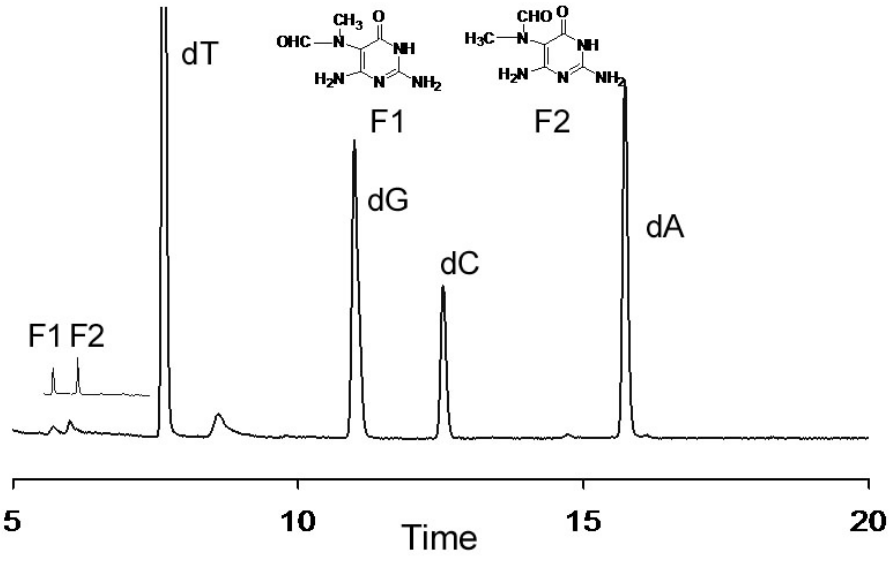

Figure S4. Enzyme digestion of oligonucleotide **1**.

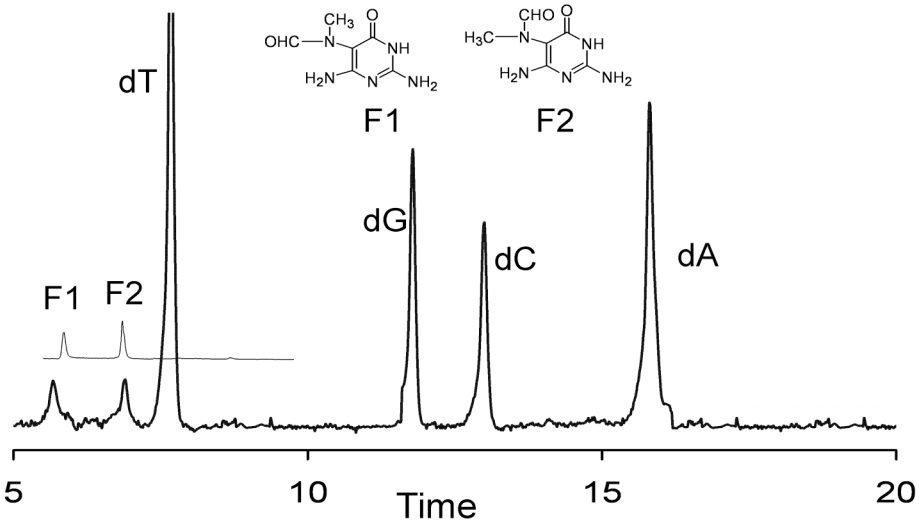

Figure S5. Enzyme digestion of oligonucleotide **2**.

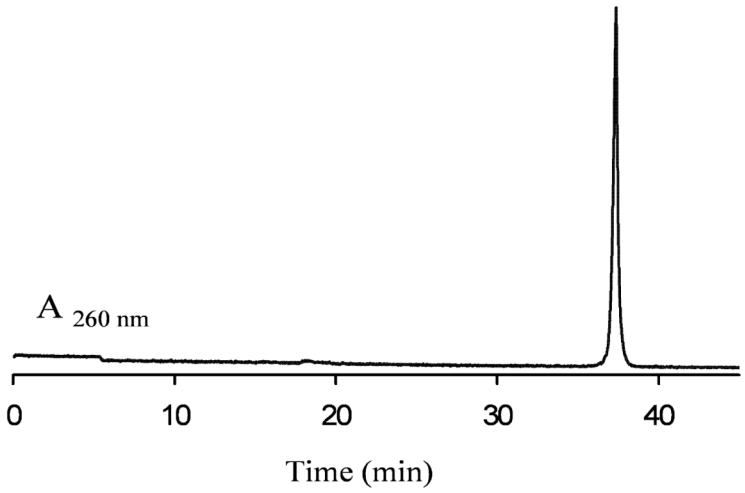

Figure S6. Capillary gel electrophoretic analysis of oligonucleotide **1**.

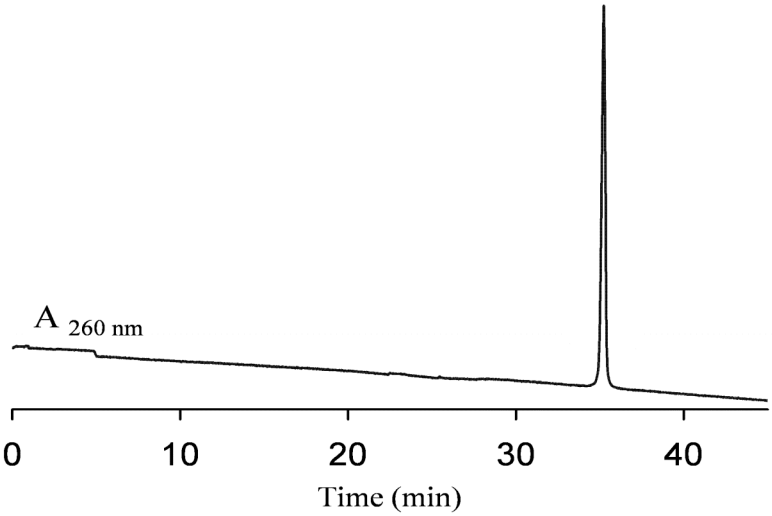

Figure S7. Capillary gel electrophoretic analysis of oligonucleotide **2**.

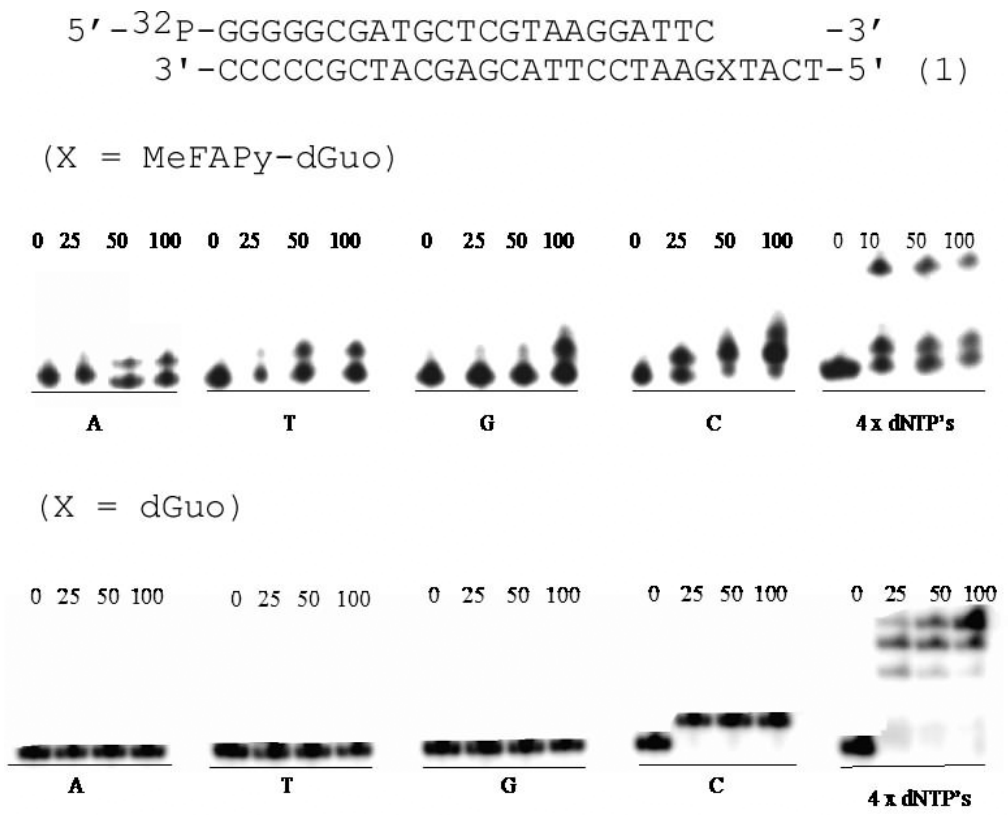

Figure S8. Single and full-length incorporation of oligonucleotides **1** catalyzed by Kf⁻.

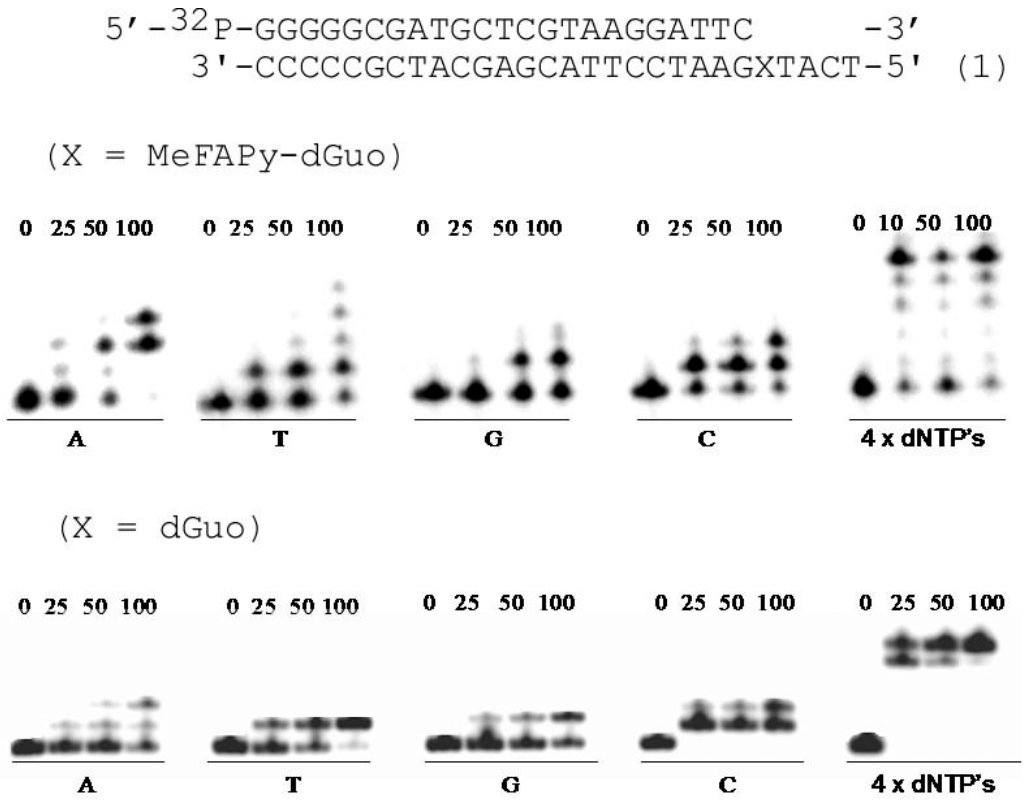

Figure S9. Single and full-length incorporation of oligonucleotides **1** catalyzed by Dpo4.

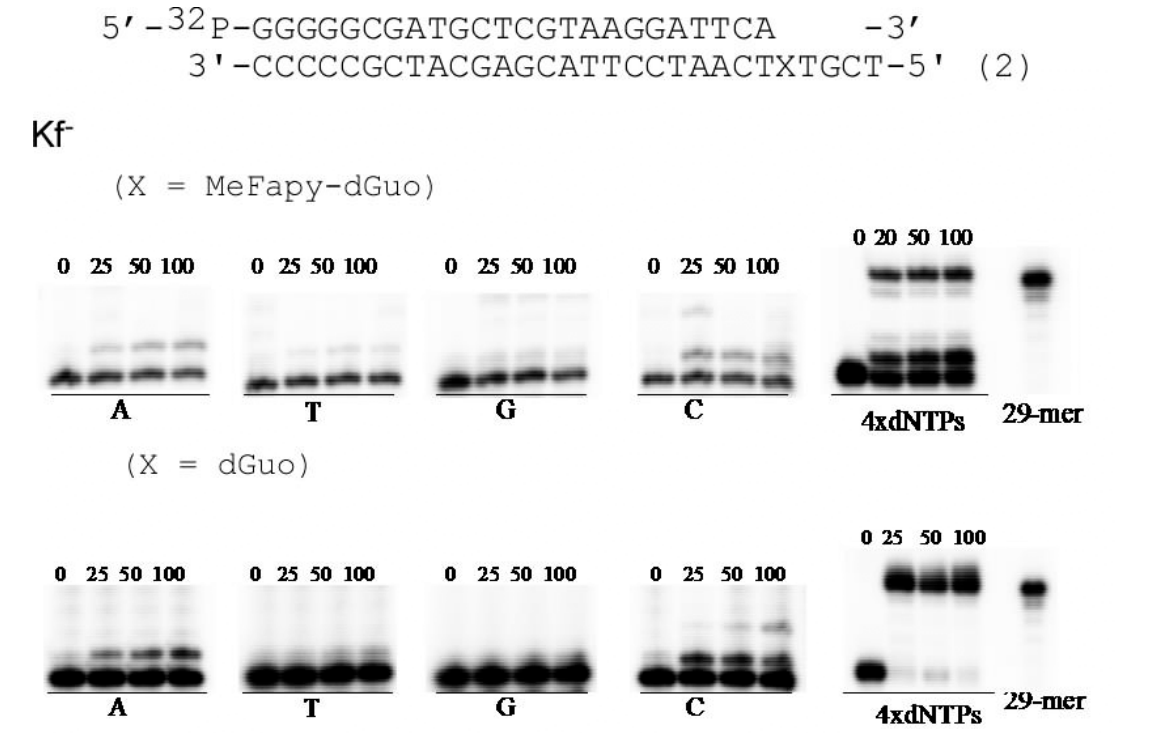

Figure S10. Single and full-length incorporation of oligonucleotides **2** catalyzed by Kf⁻.

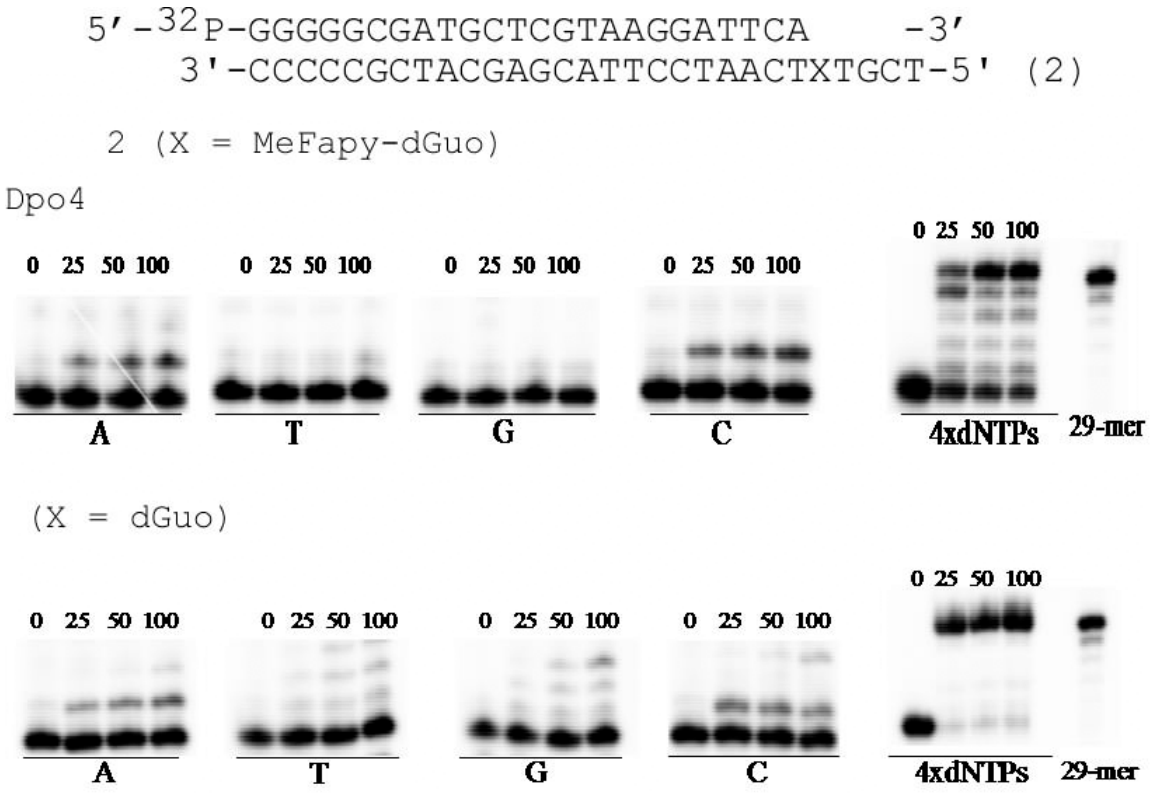

Figure S11. Single and full-length incorporation of oligonucleotides **2** catalyzed by Dpo4.

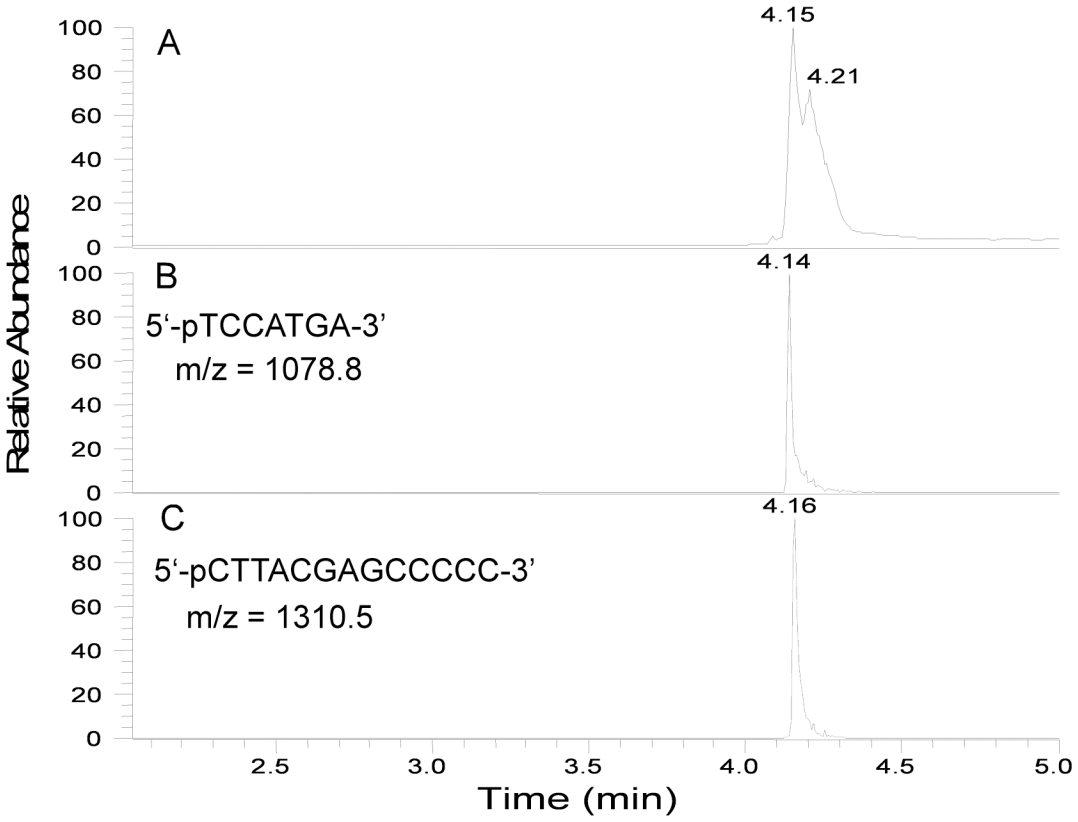

Figure S12. LC-ESI-MS/MS analysis of Dpo4 extension product from oligonucleotide **1**: TIC (A) and select ion profiles of product 5'-pTCCATGA-3' (B) and standard 5'-pCTTACGAGCCCCC-3' (C).

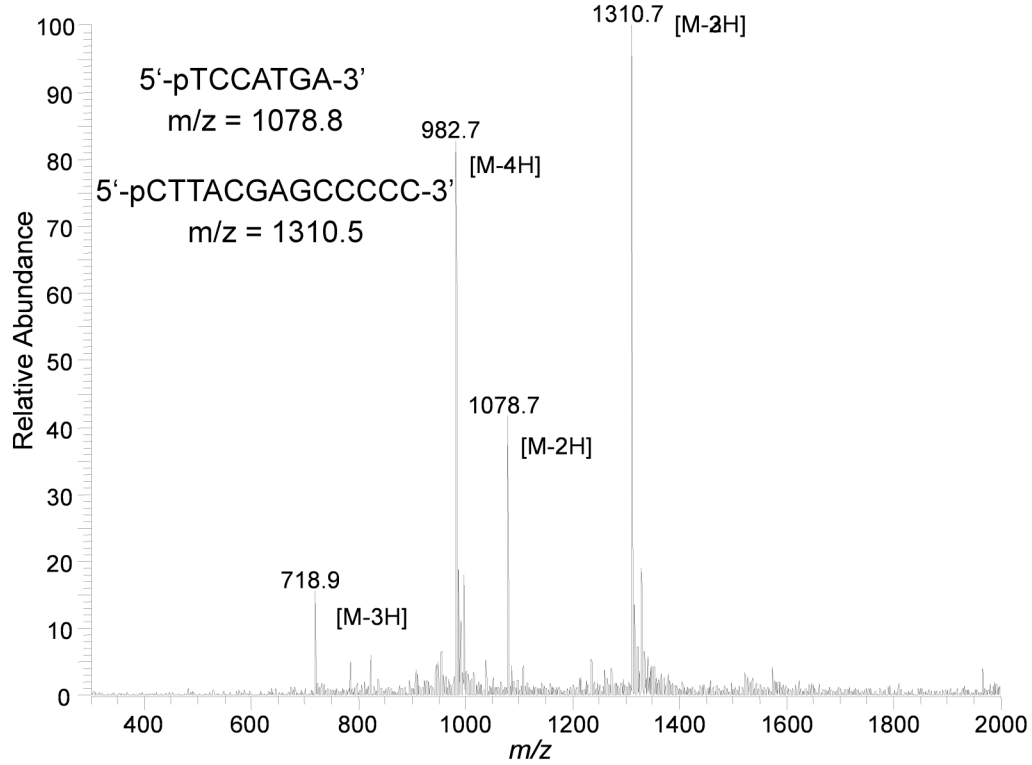

Figure S13. TIC spectrum of the *m/z* 1078.5 product from the Dpo4 extension of oligonucleotide **1**.

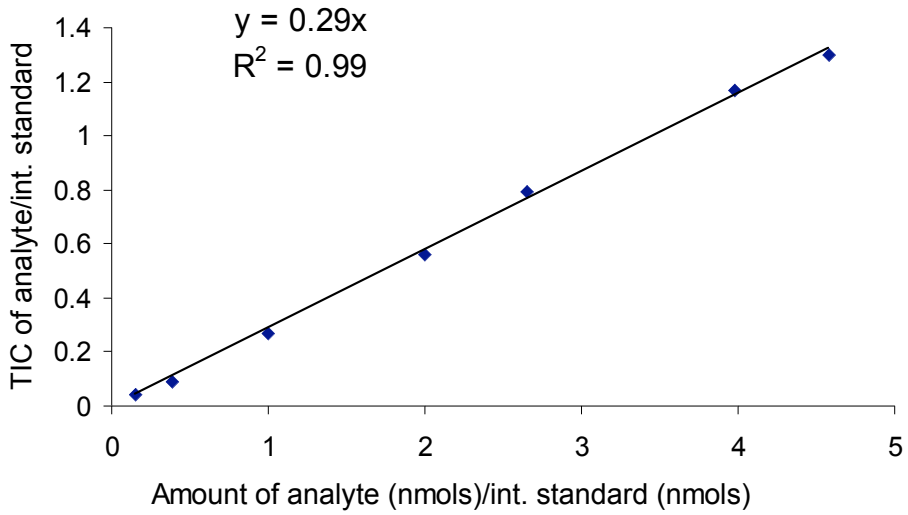

Figure S14. Calibration curve for 5'-pTCCATGA-3' vs. the internal standard 5'-pCTTACGAGCCCCC-3'.

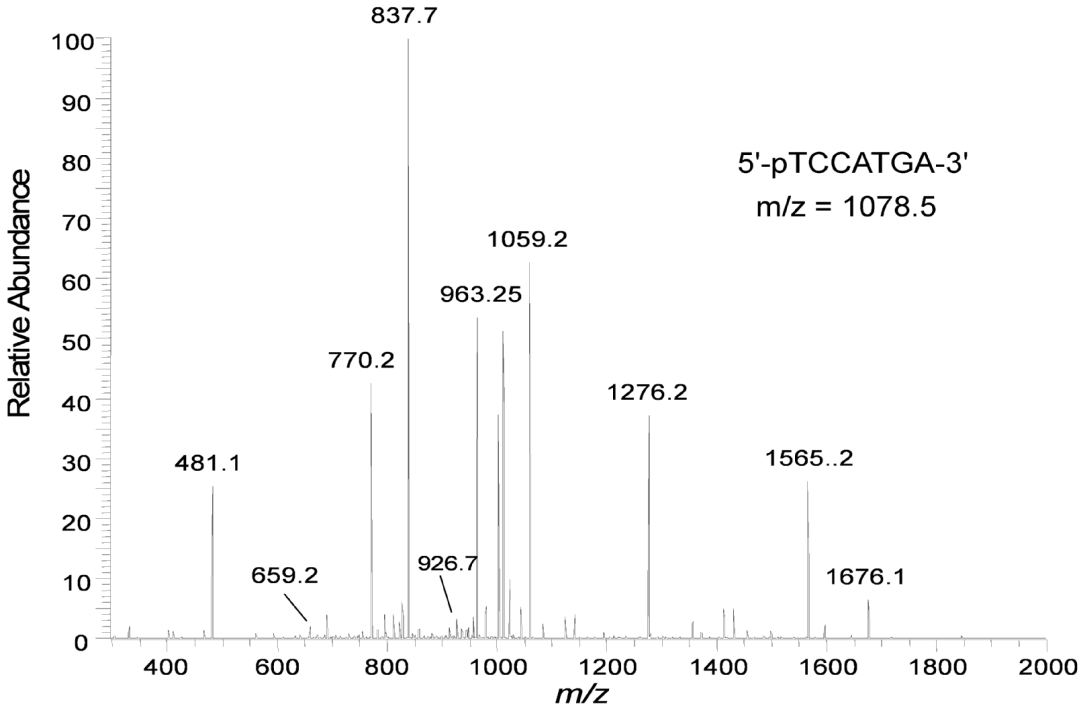

Figure S15. CID spectrum of the *m/z* 1078.5 product from the Dpo4 extension of oligonucleotide **1**. See Table 3 for CID fragment assignments.

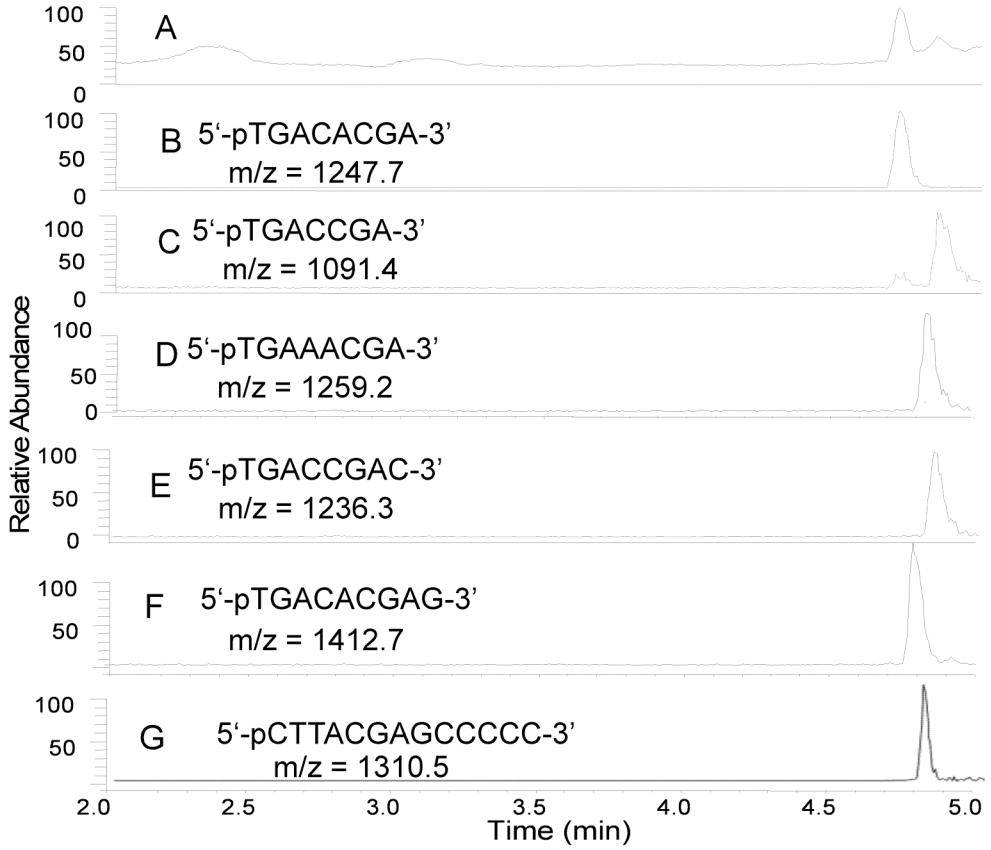

Figure S16. LC-ESI-MS/MS analysis of Kf⁻ extension products from oligonucleotide **2** : TIC (A) and select ion profiles of products 5’-pTGACACGA-3’ (B), 5’-pTGACCGA-3’ (C) , 5’-pTGAAACGA-3’ (D), 5’-pTGACCGAC-3’ (E), and 5’-pTGACACGAG-3’ (F) and standard 5’-pCTTACGAGCCCC-3’ (G).

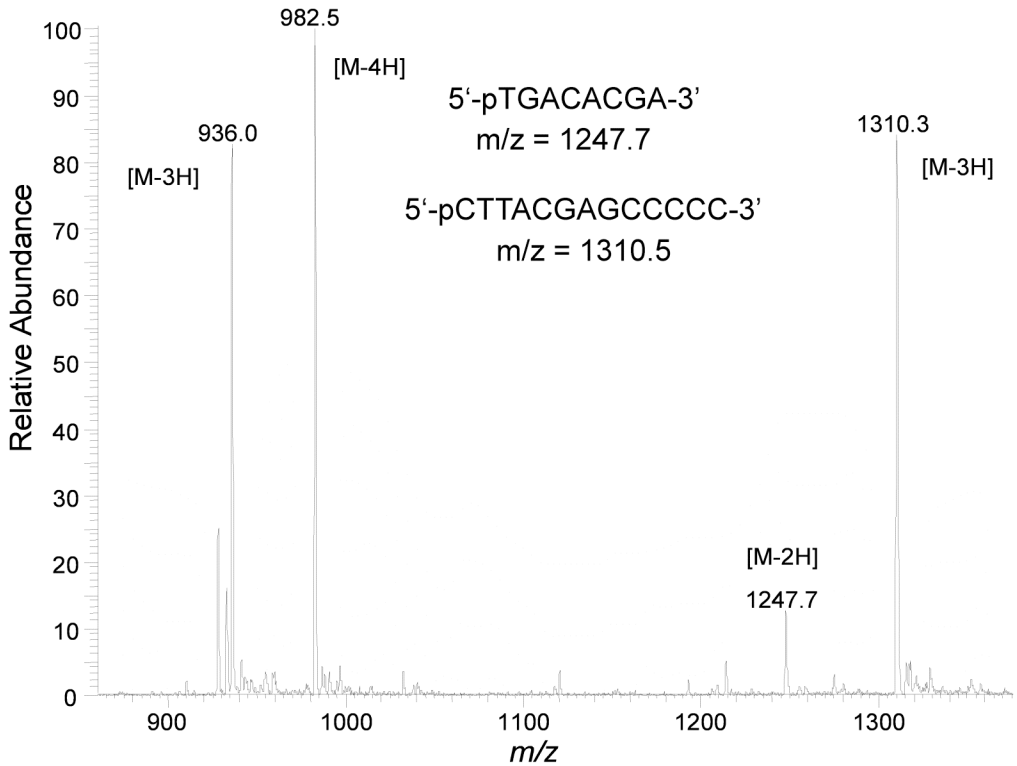

Figure S17. TIC spectrum of the Kf⁻ extension products from oligonucleotide **2**.

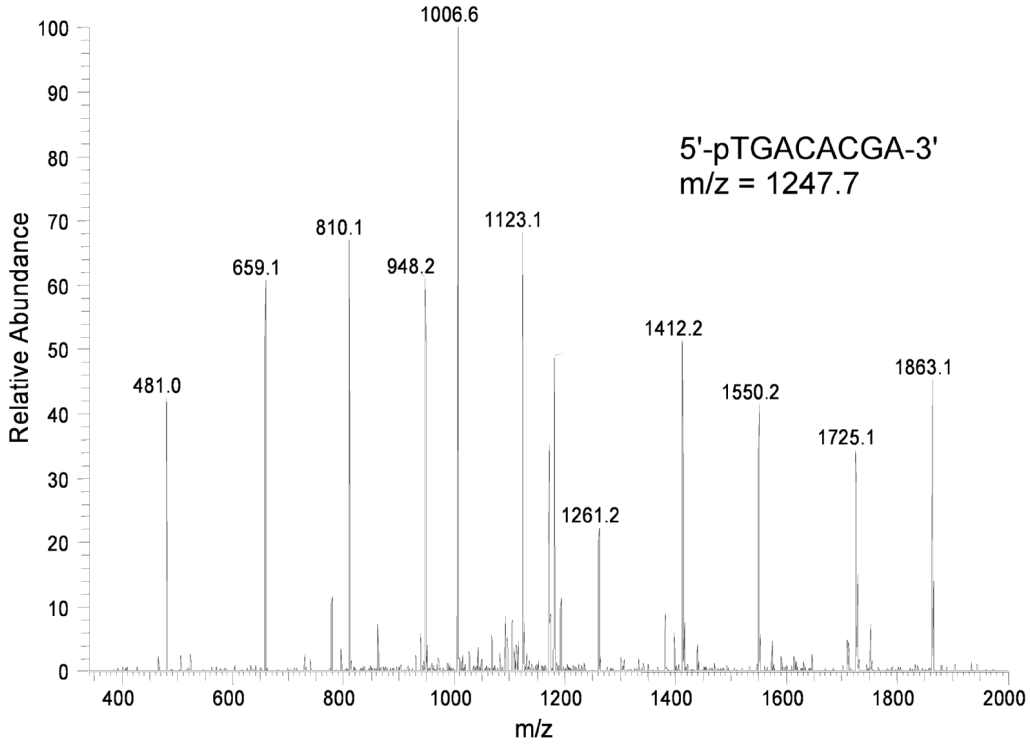

Figure S18. CID spectrum of the *m/z* 1247.7 product from the Kf⁻ extension of oligonucleotide **2**.

Table S1. Observed and calculated CID fragmentation of 5'-pTGACACGA-3'

Fragment assignment	Observed	Theoretical
5'-pT (a_2-B)	481.1	481
5'-pTG (a_3-B)	810.1	810
5'-pTGA (a_4-B)	1123.1	1123.1
5'-pTGAC (a_5-B)	1412.2	1412.1
5'-pTGACA (a_6-B)	1725.1	1725.2
5'-pTGACAC (a_7-B, -2)	1006.6	1006.6
pACACGA-3' (w_6)	1863.1	1863.3
pCACGA-3' (w_5)	1550.2	1550.2
pACGA-3' (w_4)	1261.2	1261.2
pCGA-3' (w_3)	948.2	948.1
pGA-3' (w_2)	659.1	659.1

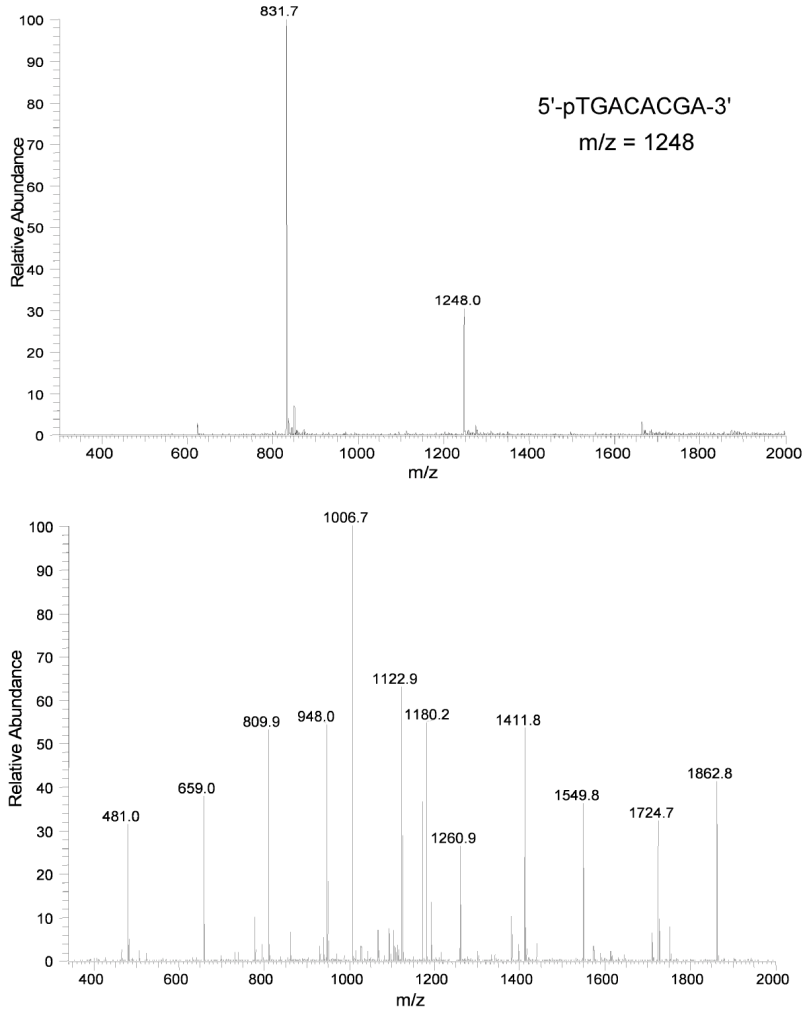

Figure S19. TIC (top) and CID (bottom) spectra of an authentic sample of 5'-pTGACACGA-3'

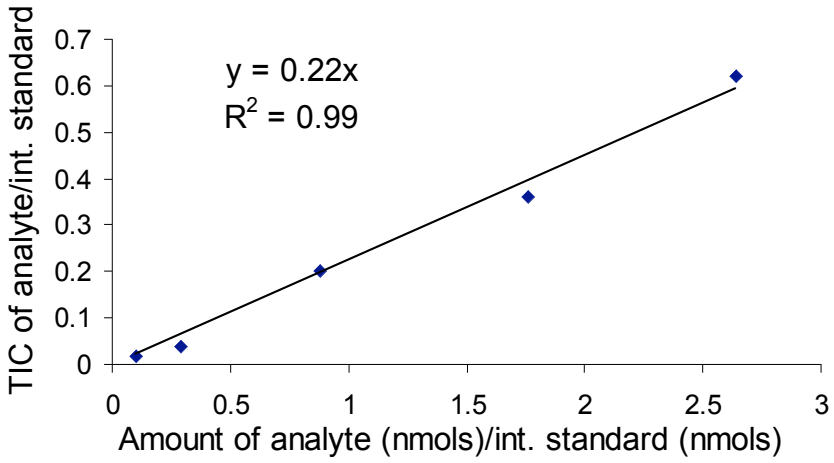

Figure S20. Calibration curve for 5'-pTGACACGA-3' vs. the internal standard 5'-pCTTACGAGCCCCC-3'

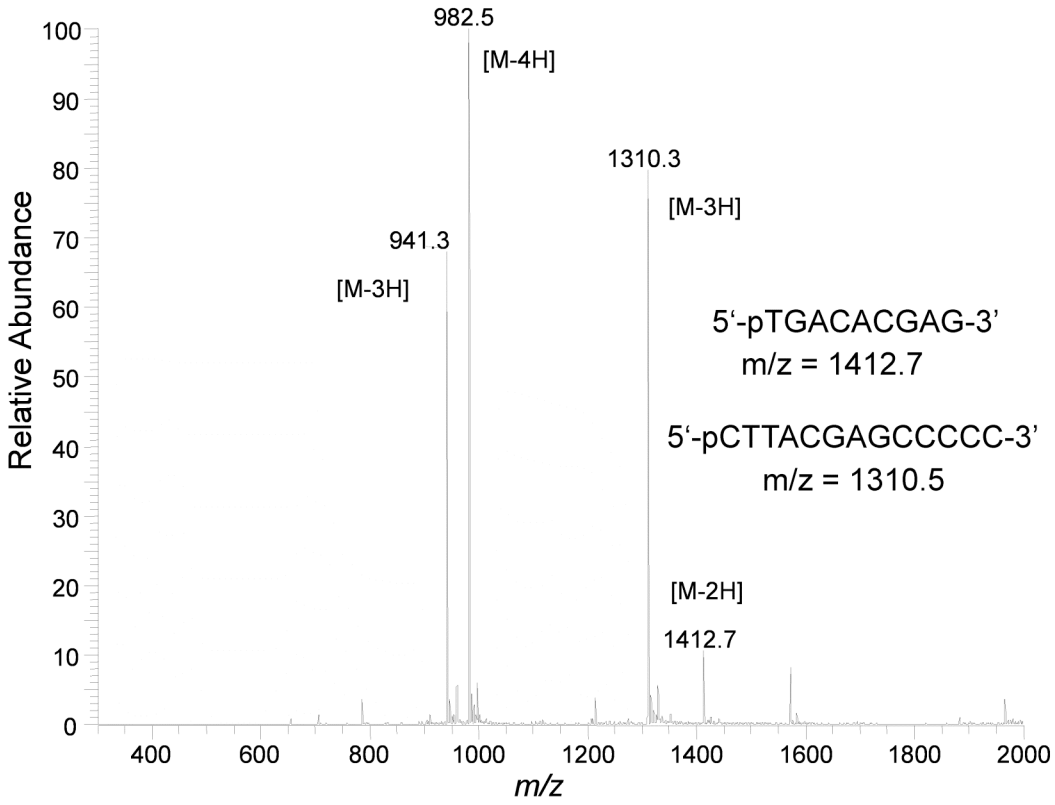

Figure S21. TIC spectrum of the Kf⁻ extension products from oligonucleotide **2**.

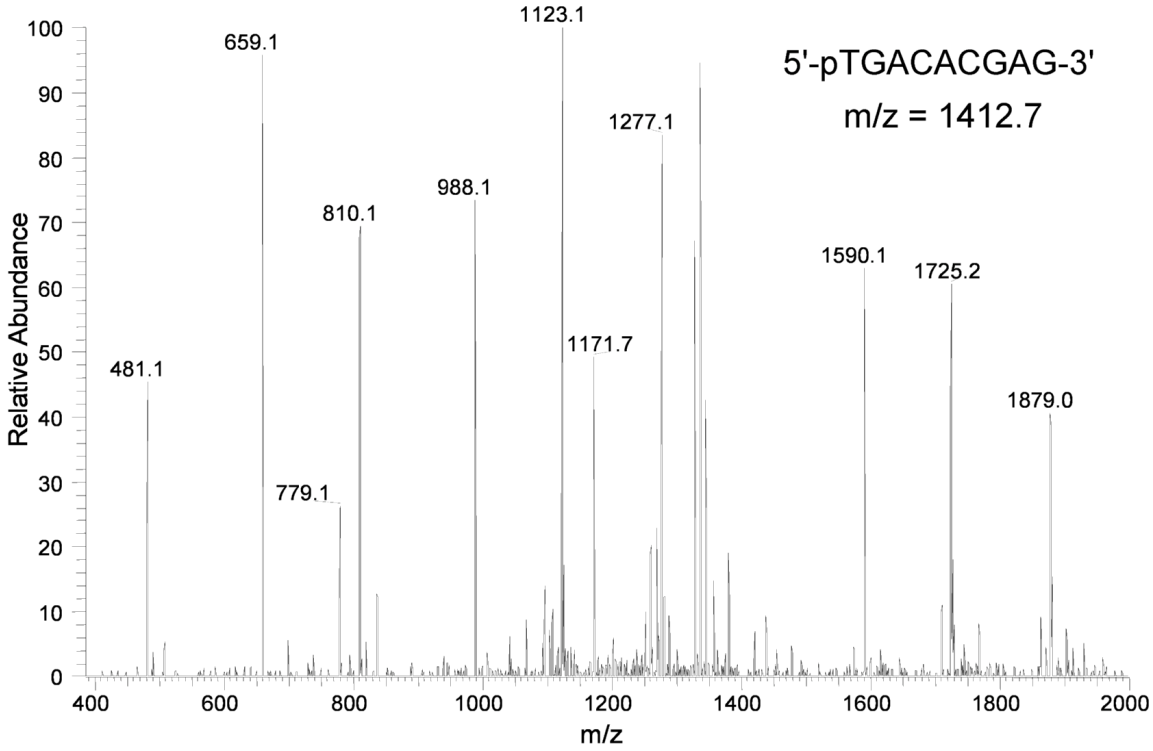

Figure S22. CID spectrum of the *m/z* 1412.8 product from the Kf⁻ extension of oligonucleotide **2**.

Table S2. Observed and calculated CID fragmentation of 5’-pTGACACGAG-3

Fragment assignment	Observed	Theoretical
5'-pT (a_2-B)	480.1	481
5'-pTG (a_3-B)	810.1	810
5'-pTGA (a_4-B)	1123.1	1123.1
5'-pTGACA (a_6-B)	1725.2	1725.2
5'-pTGACACGA (a_8-B, -2)	1171.7	1171.1
5'-pTGACACGA (a_8-B, -3)	779.1	780.4
pCACGAG-3' (w_6)	1879	1879.3
pACGAG-3' (w_5)	1590.1	1590.2
pCGAG-3' (w_4)	1277.1	1277.2
pGAG-3' (w_3)	988.1	988.1
pAG-3' (w_2)	659.1	659.1

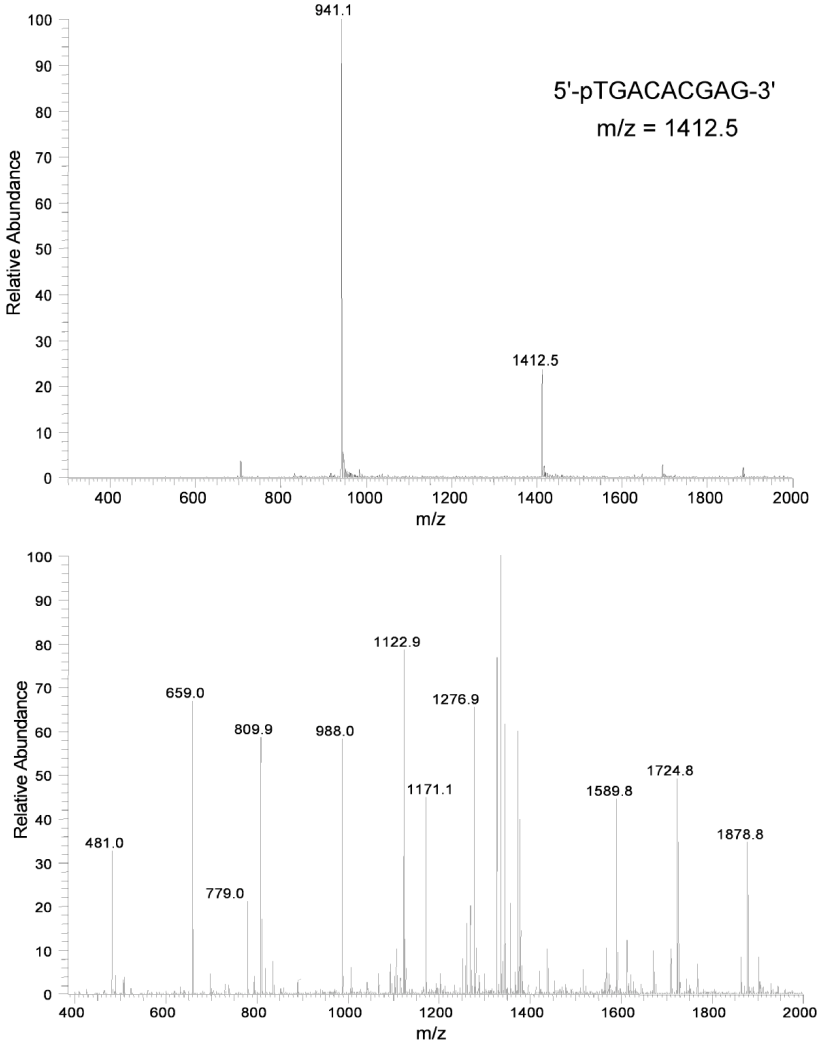

Figure S23. TIC (top) and CID (bottom) spectra of an authentic sample of 5’-pTGACACGAG-3’

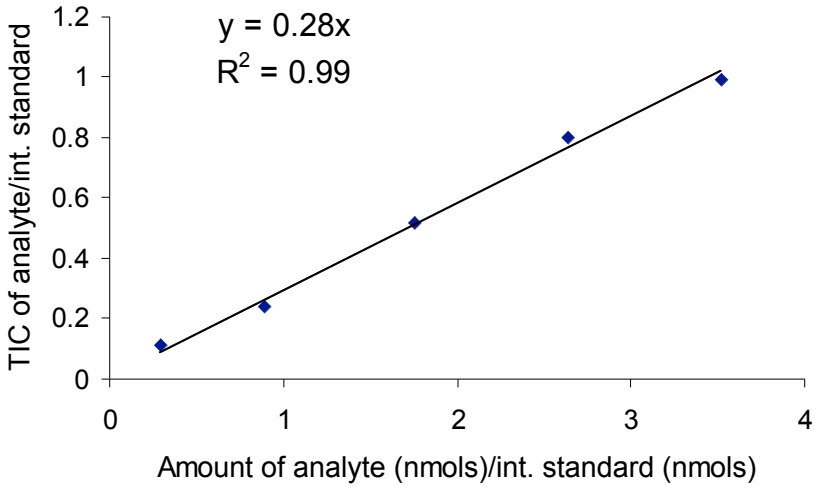

Figure S24. Calibration curve for 5'-pTGACACGAG-3'vs. the internal standard 5'-pCTTACGAGCCCCC-3'

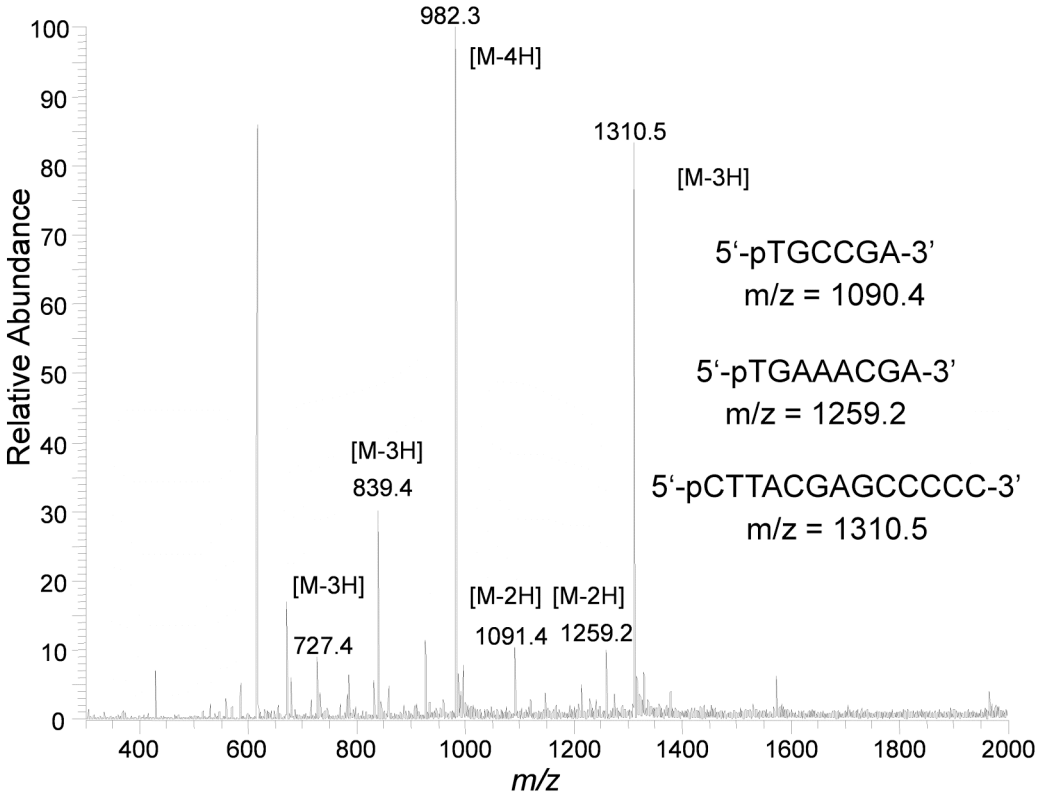

Figure S25. TIC spectrum of the Kf⁻ extension products from oligonucleotide **2**.

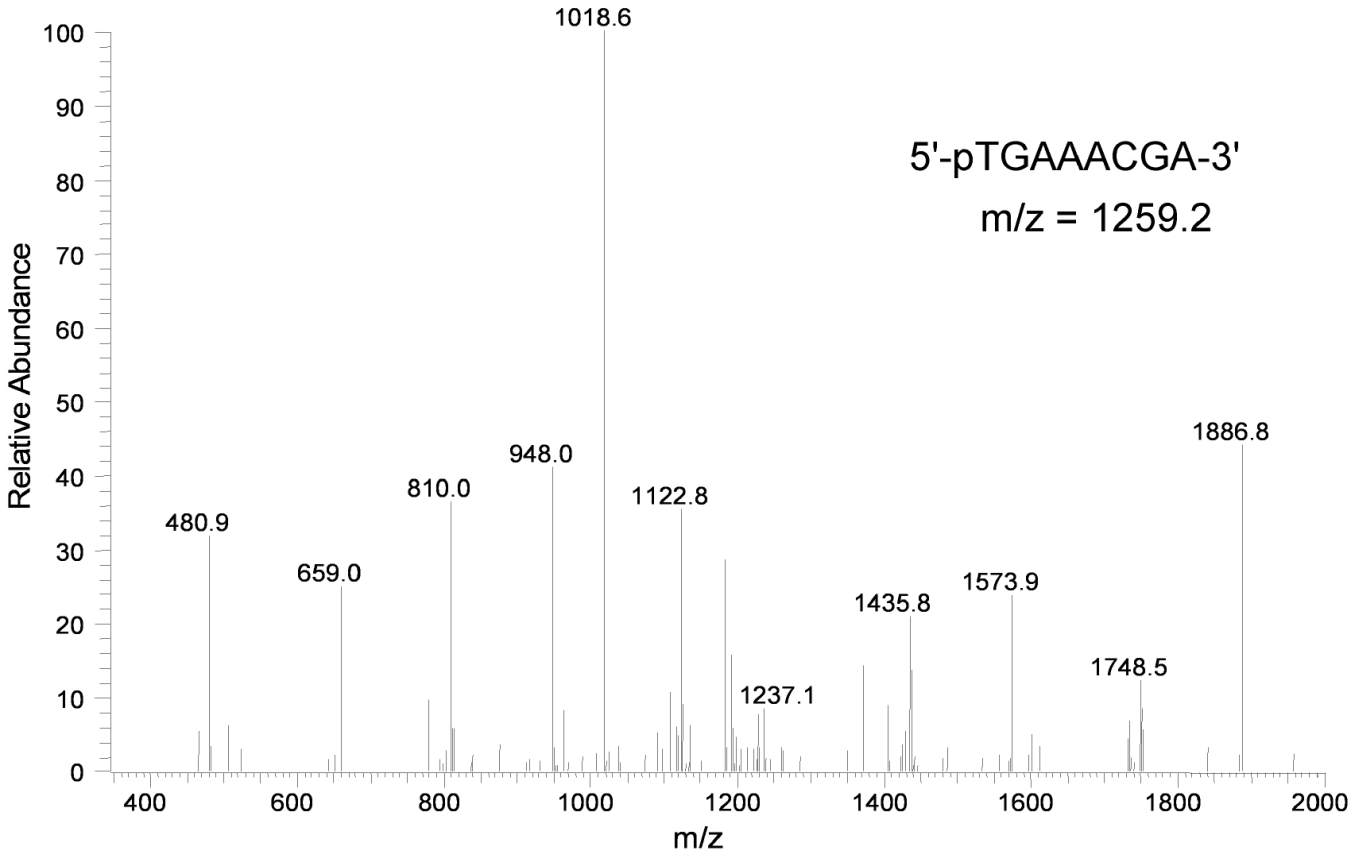

Figure S26. CID spectrum of the *m/z* 1259.2 product from the Kf⁻ extension of oligonucleotide **2**.

Table S3. Observed and calculated CID fragmentation of 5'-pTGAAACGA-3

Fragment assignment	Observed	Theoretical
5'-pT (a_2-B)	480.9	481
5'-pTG (a_3-B)	810	810
5'-pTGA (a_4-B)	1122.8	1123.1
5'-pTGAA (a_5-B)	1435.8	1436.9
5'-pTGAAA (a_6-B)	1748.5	1750.11
5'-pTGAAA (a_6-B, -2)	874.4	874.55
5'-pTGAAAC (a7-B, -2)	1018.6	1019.14
pAAACGA-3' (w_5)	1886.8	1888.2
pAACGA-3' (w_5)	1573.9	1575.03
pCGA-3' (w_3)	948	948.61
pGA-3' (w_2)	659	659.42

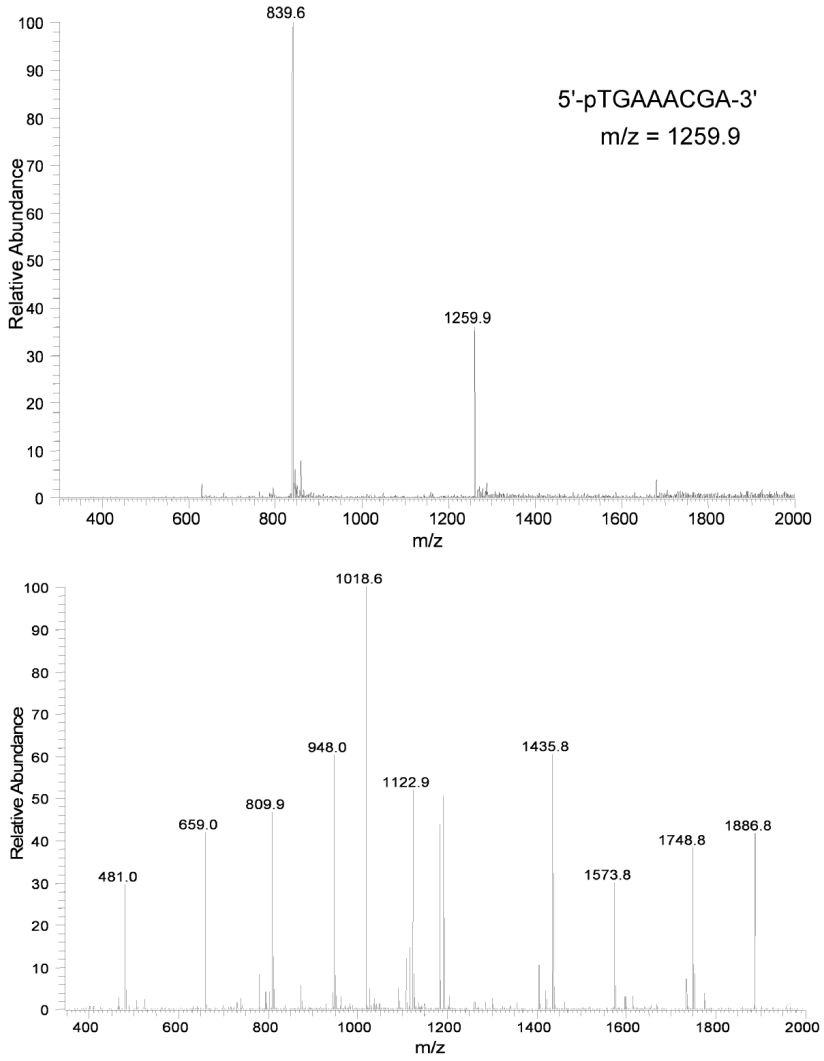

Figure S27. TIC (top) and CID (bottom) spectra of an authentic sample of 5'-pTGAAACGA-3'

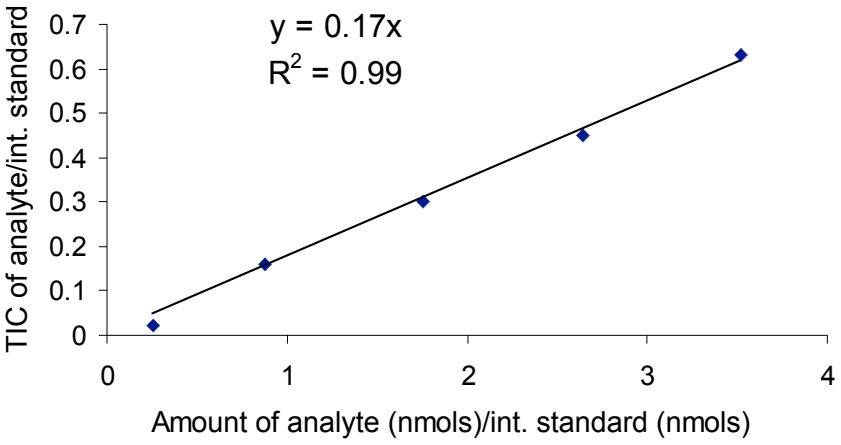

Figure S28. Calibration curve for 5'-pTGAAACGA-3' vs. the internal standard 5'-pCTTACGAGCCCCC-3'

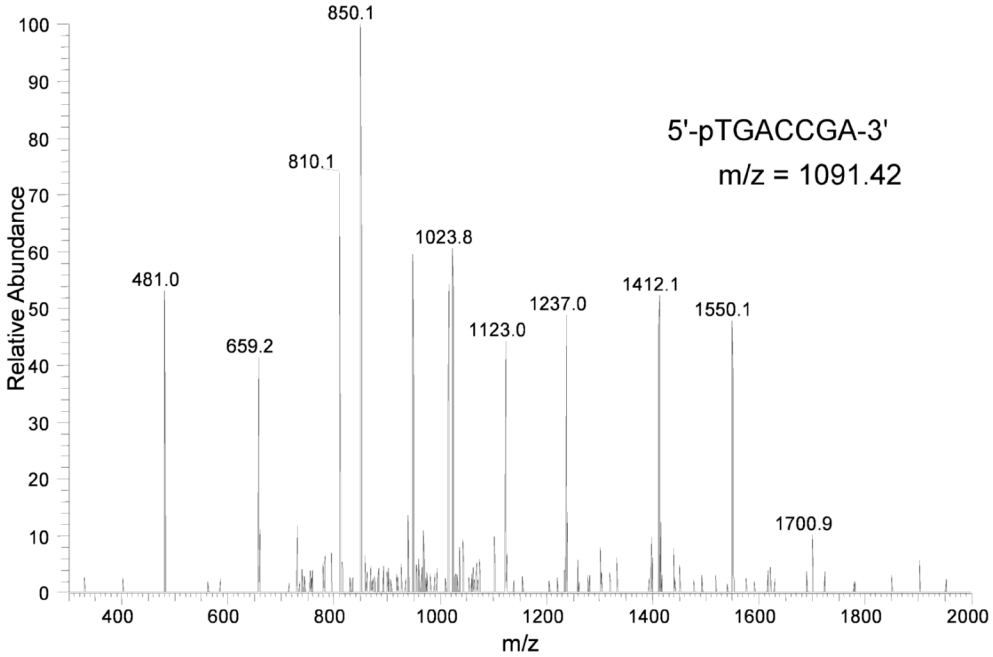

Figure S29. CID spectrum of the *m/z* 1091.42 product from the Kf^- extension of oligonucleotide **2**. See Table 4 for fragment assignments.

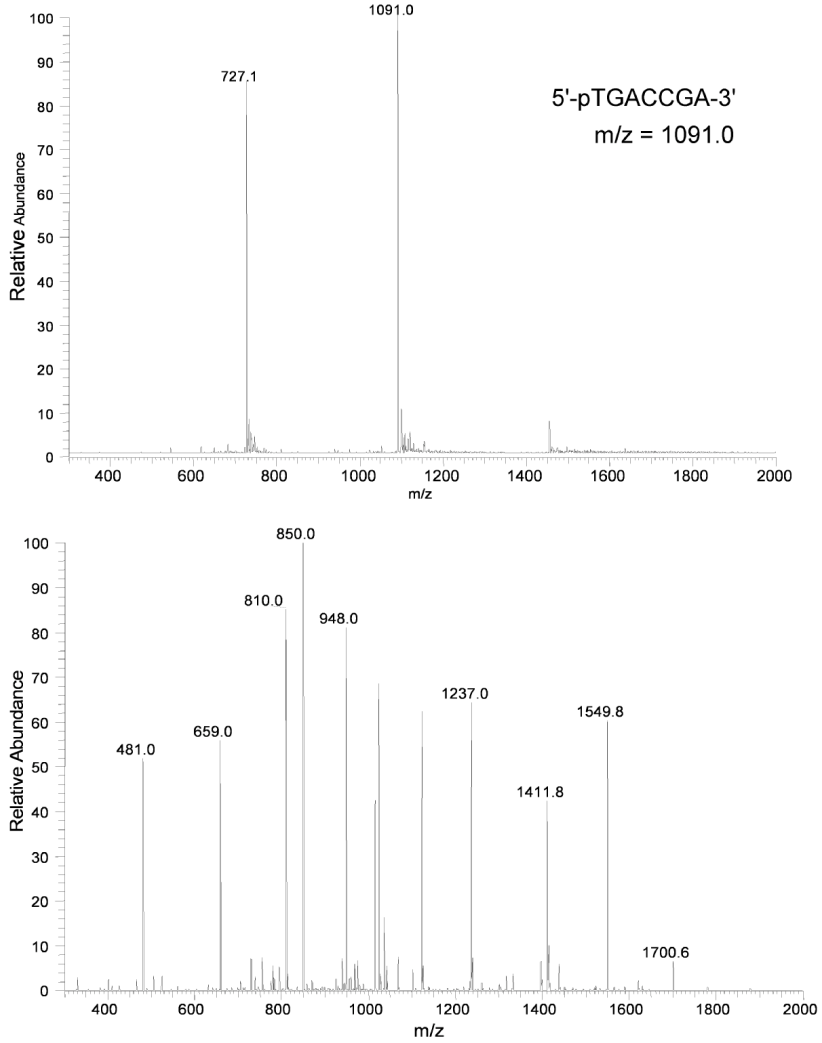

Figure S30. TIC (top) and CID (bottom) spectra of an authentic sample of 5'-pTGACCGA-3'

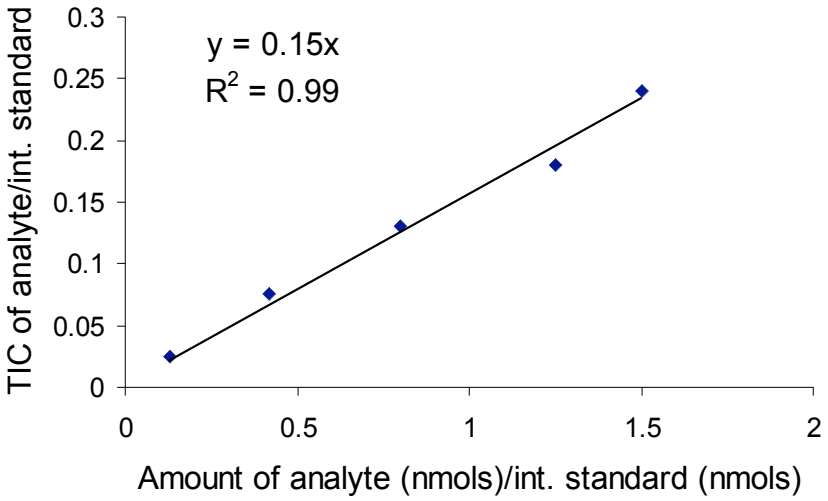

Figure S31. Calibration curve for 5'-pTGACCGA-3'vs. the internal standard 5'-pCTTACGAGCCCCC-3'.

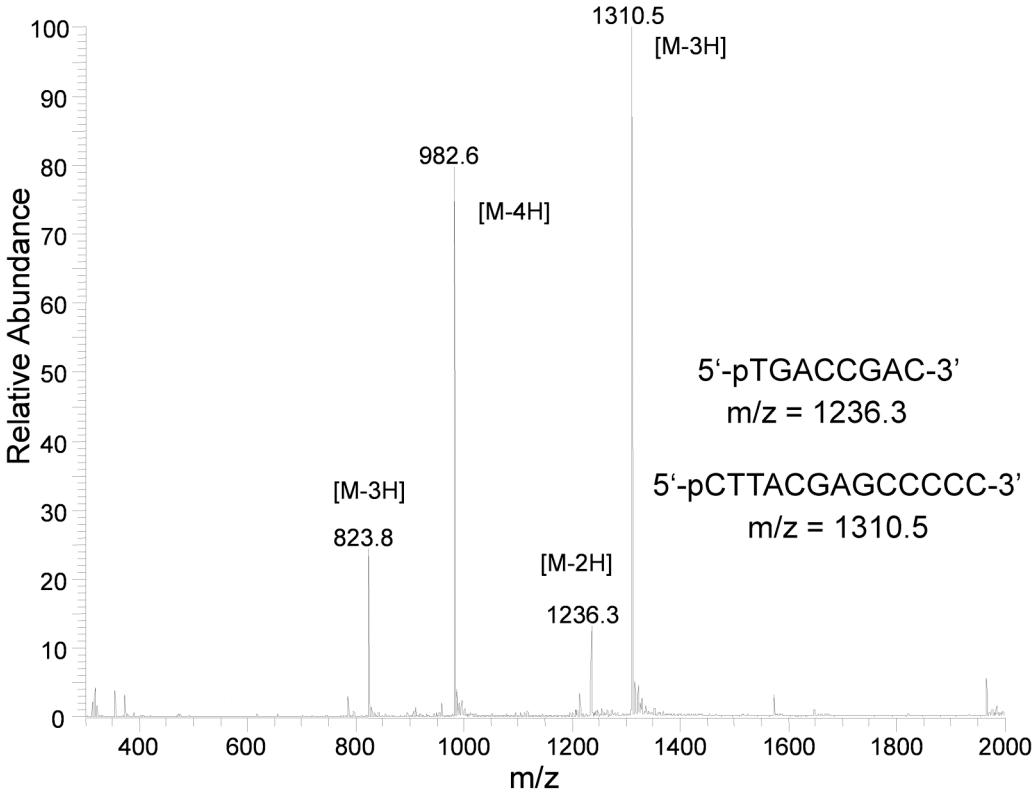

Figure S32. TIC spectrum of the Kf⁻ extension products from oligonucleotide **2**.

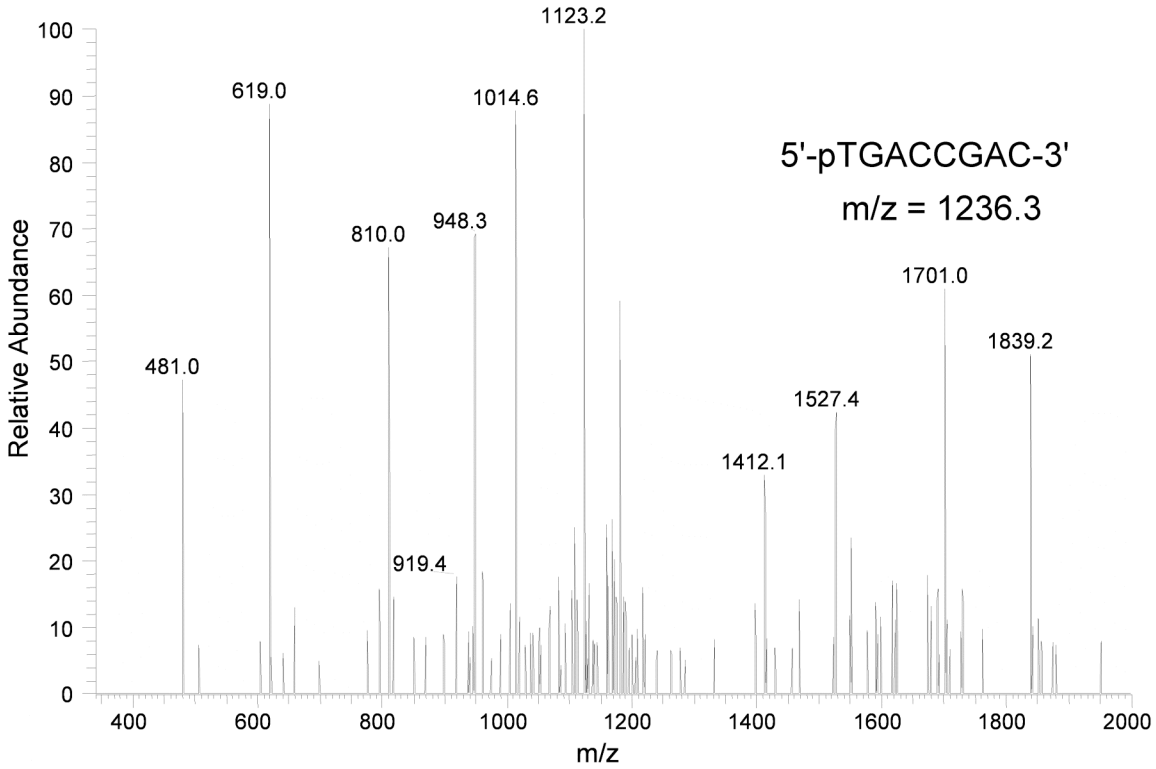

Figure S33. CID spectrum of the *m/z* 1236.3 product from the Kf⁻ extension of oligonucleotide **2**.

Table S4. Observed and calculated CID fragmentation of 5'-pTGACCGAC-3

Fragment assignment	Observed	Theoretical
5'-pT (a_2-B)	481	481
5'-pTG (a_3-B)	810	810
5'-pTGA (a_4-B)	1123.2	1123.1
5'-pTGAC (a_5-B)	1412.1	1412.1
5'-pTGACC (a_6-B)	1701	1702
5'-pTGACCG (a_7-B, -2)	1014.6	1015.1
pACCGAC-3' (w_6)	1839.2	1840.1
pACCGAC-3' (w_6, -2)	919.4	919.5
pCCGAC-3' (w_5)	1527.4	1526.9
pCGAC-3' (w_4)	619	618.3
pGAC-3' (w_3)	948.3	948.6
pAC-3' (w_2)	619	619.4

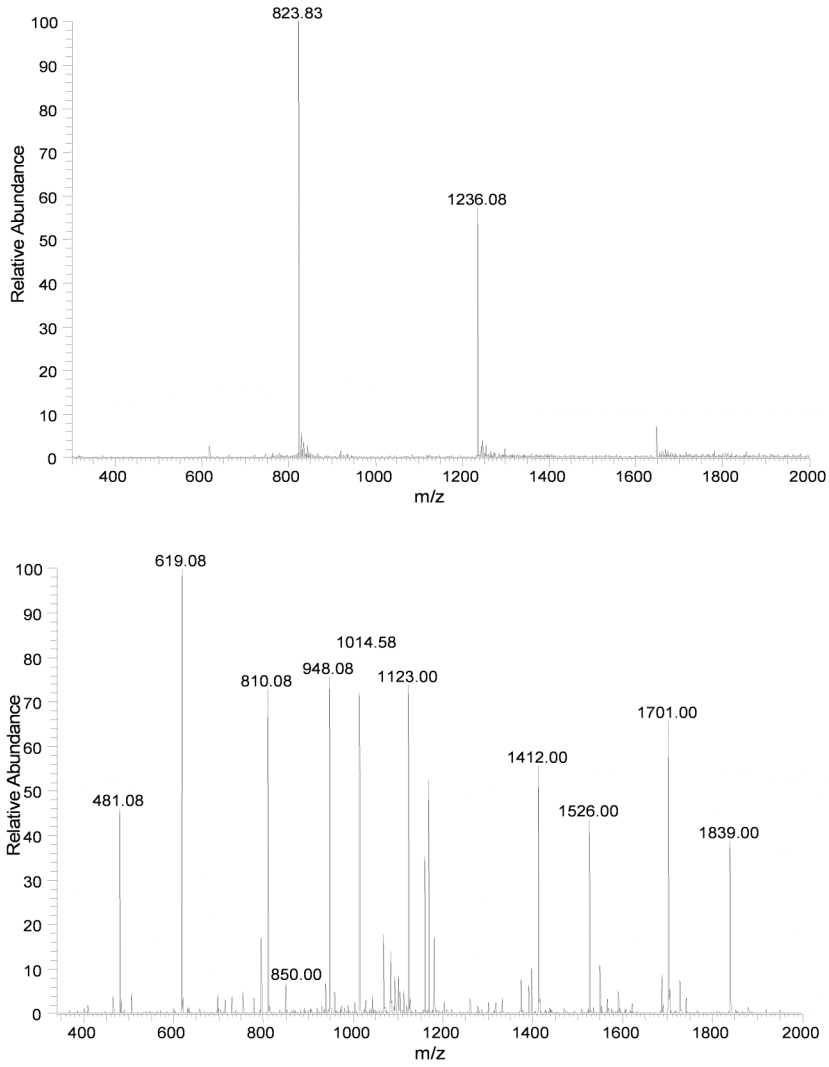

Figure S34. TIC (top) and CID (bottom) spectra of an authentic sample of 5'-pTGACCGAC-3'

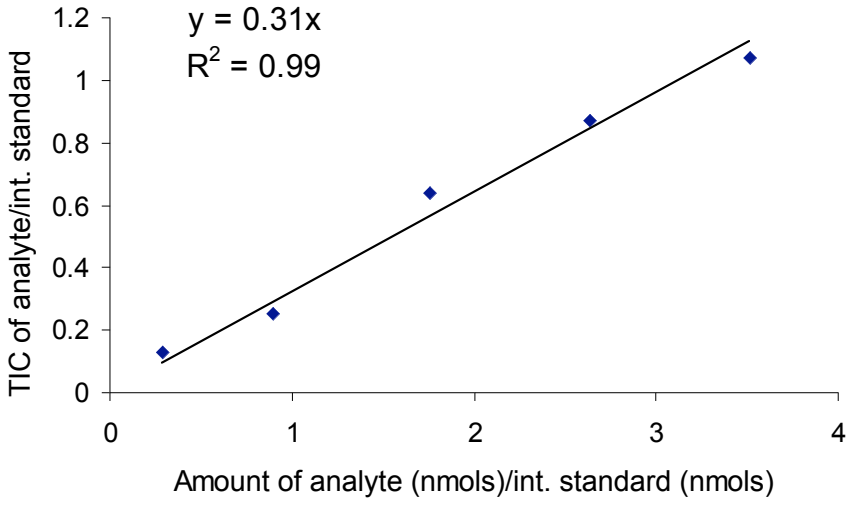

Figure S35. Calibration curve for 5'-pTGACCGAC-3' vs the internal standard 5'-pCTTACGAGCCCCC-3'.

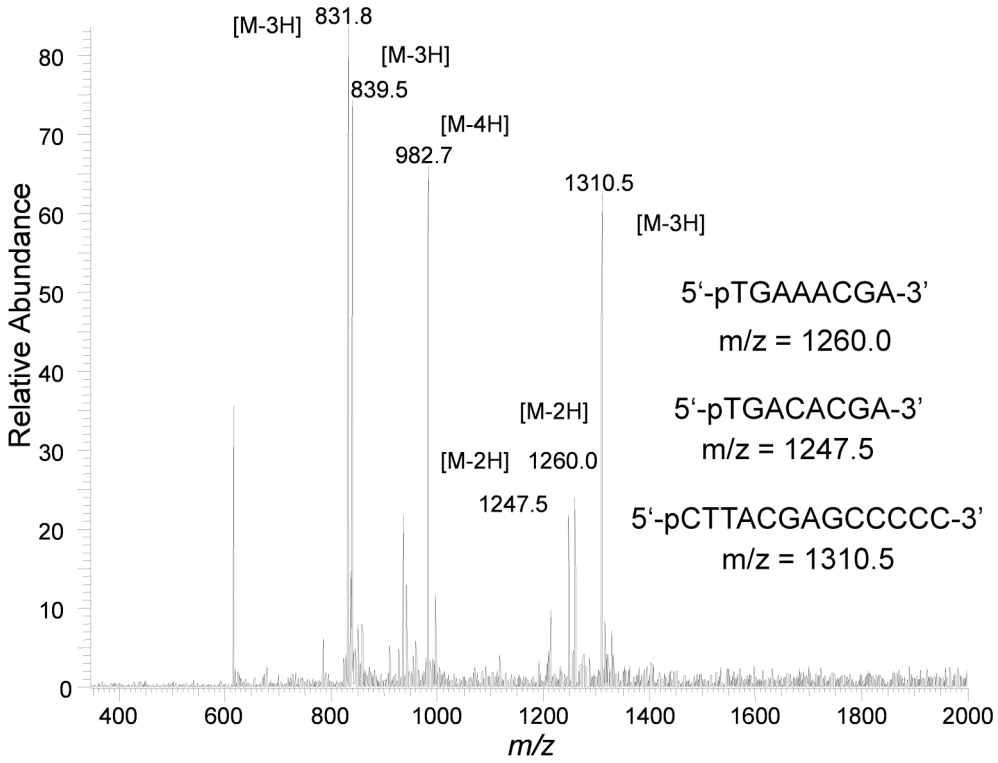

Figure S36. TIC spectrum of the Dpo4 extension products from oligonucleotide **2**.

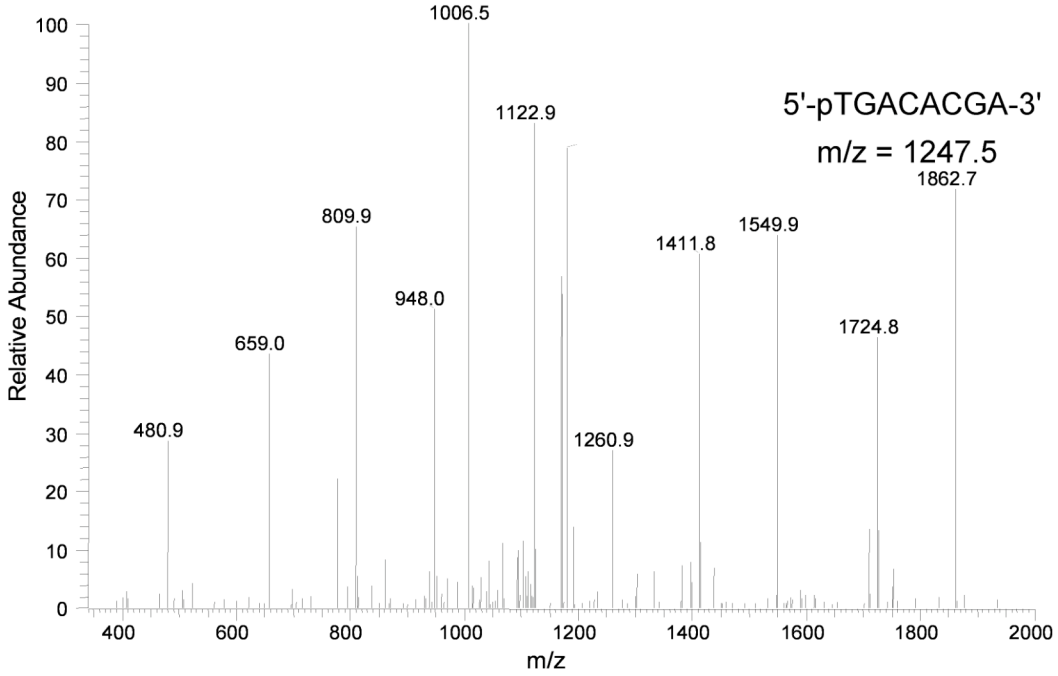

Figure S37. CID spectrum of the *m/z* 1247.5 product from the Dpo4 extension of oligonucleotide **2**. See Table S1 for fragment assignments.

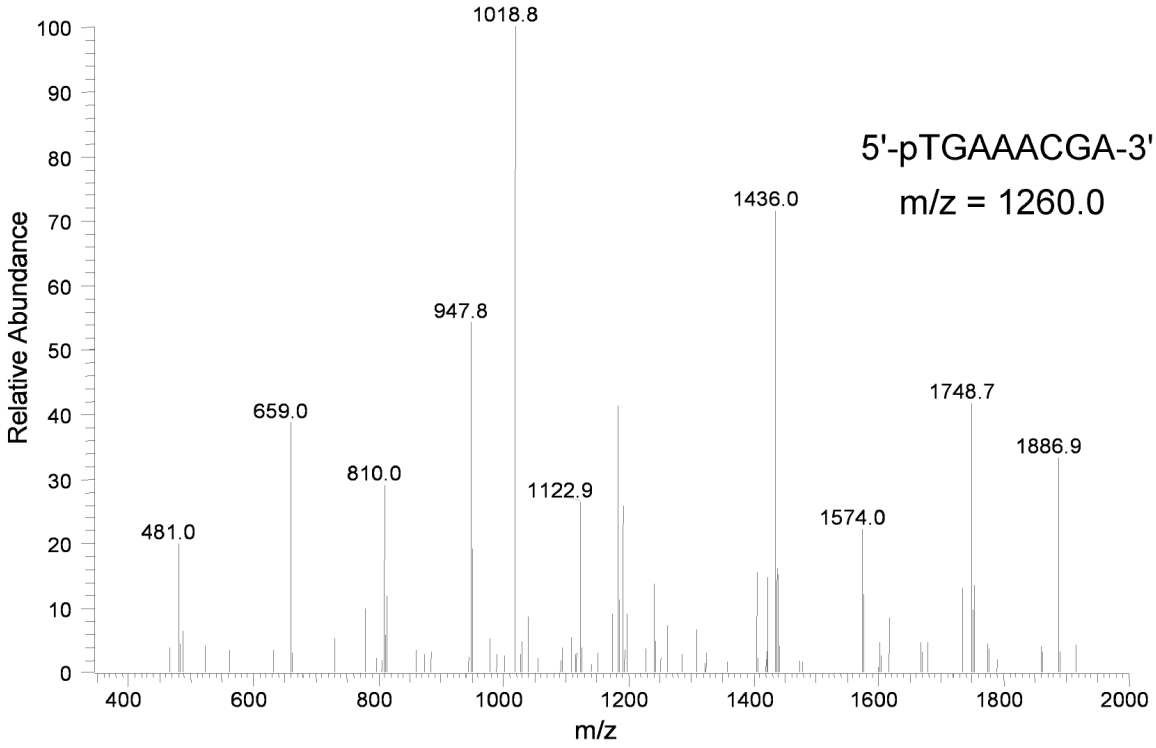

Figure S38. CID spectrum of the *m/z* 1260.0 product from the Dpo4 extension of oligonucleotide **2**.

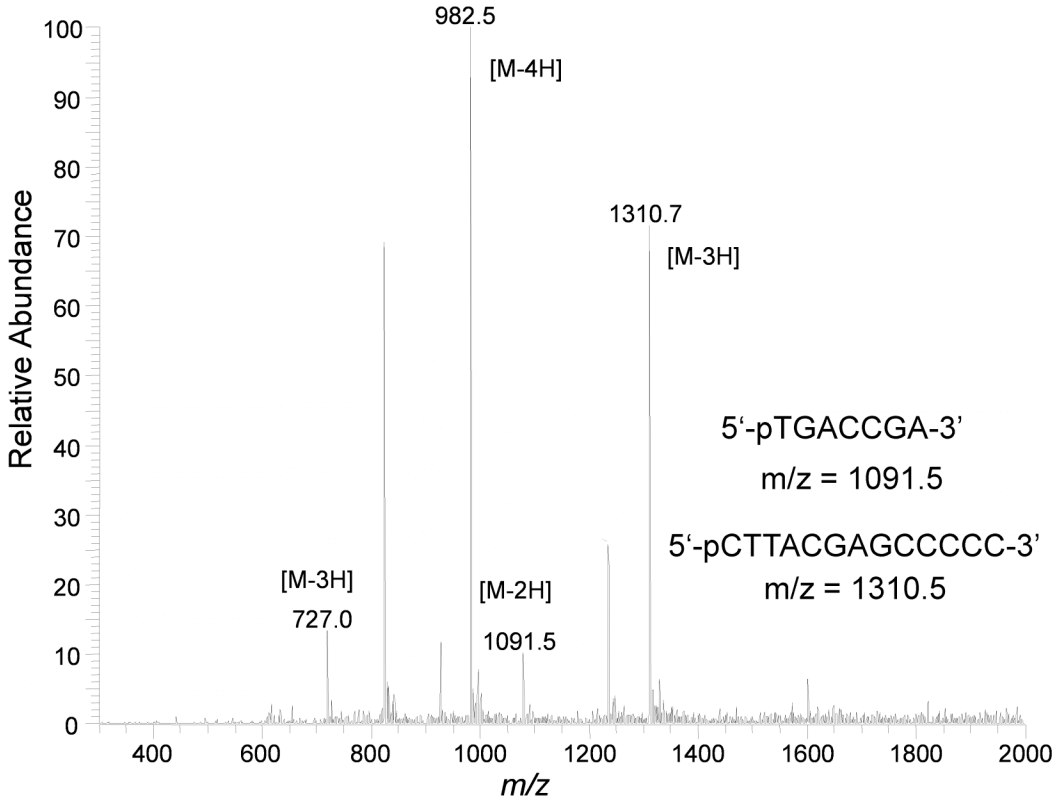

Figure S39. TIC spectrum of the Dpo4 extension products from oligonucleotide **2**.

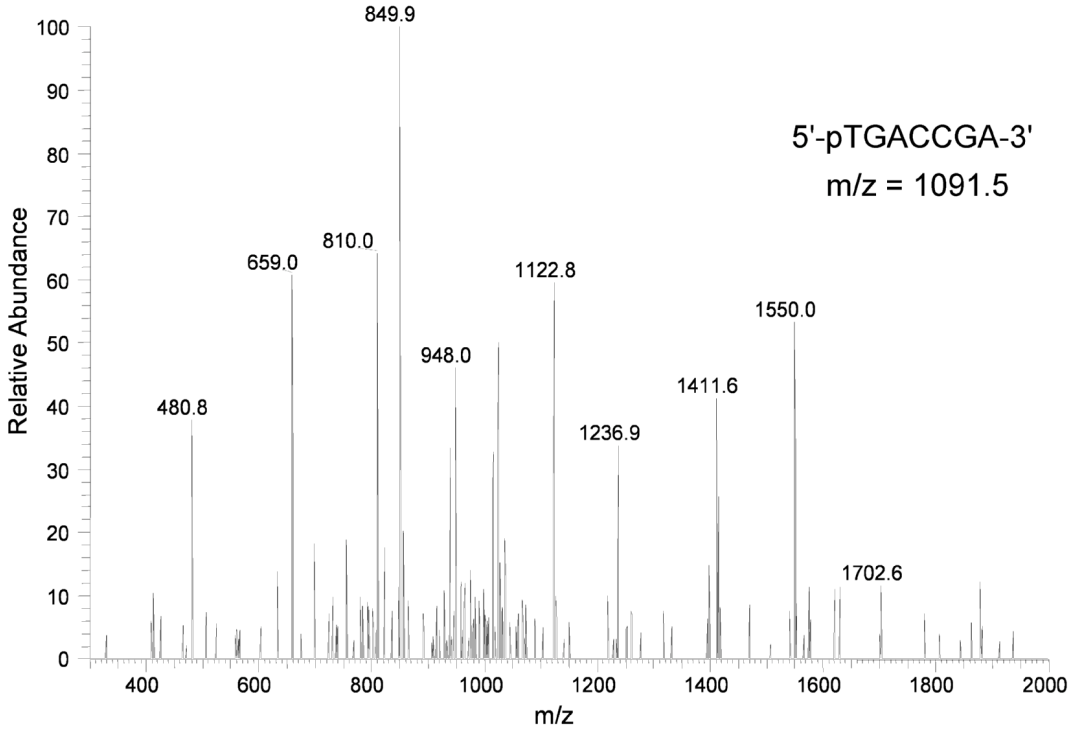

Figure S40. CID spectrum of the *m/z* 1091.5 product from the Dpo4 extension of oligonucleotide **2**. See Table 4 for fragment assignments.