Supporting Information for:

Translesion synthesis past the C8- and N^2-deoxyguanosine adducts of the dietary mutagen 2-amino-3-methylimidazo[4,5-*f*]quinoline (IQ) in the *Nar*I recognition sequence by bacterial DNA polymerases.

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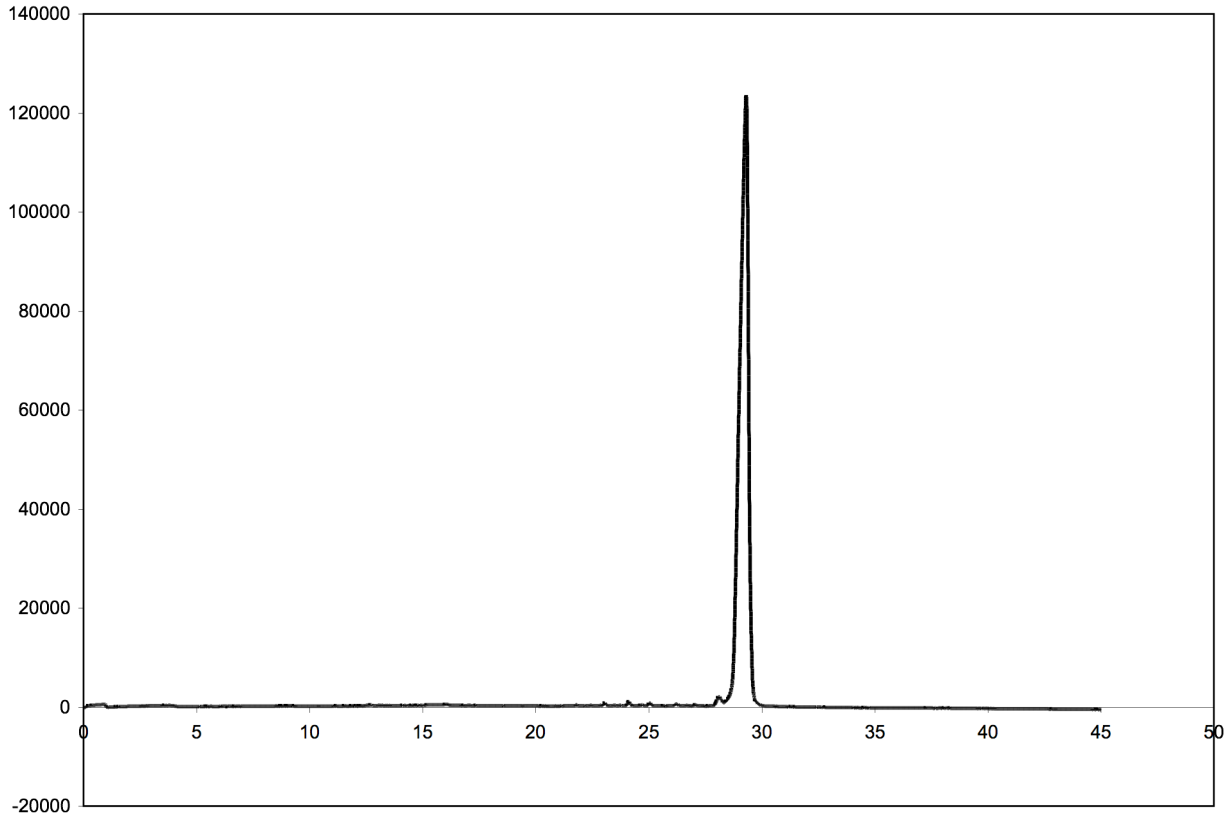

Figure S1. CGE analysis of oligonucleotide **1b**.

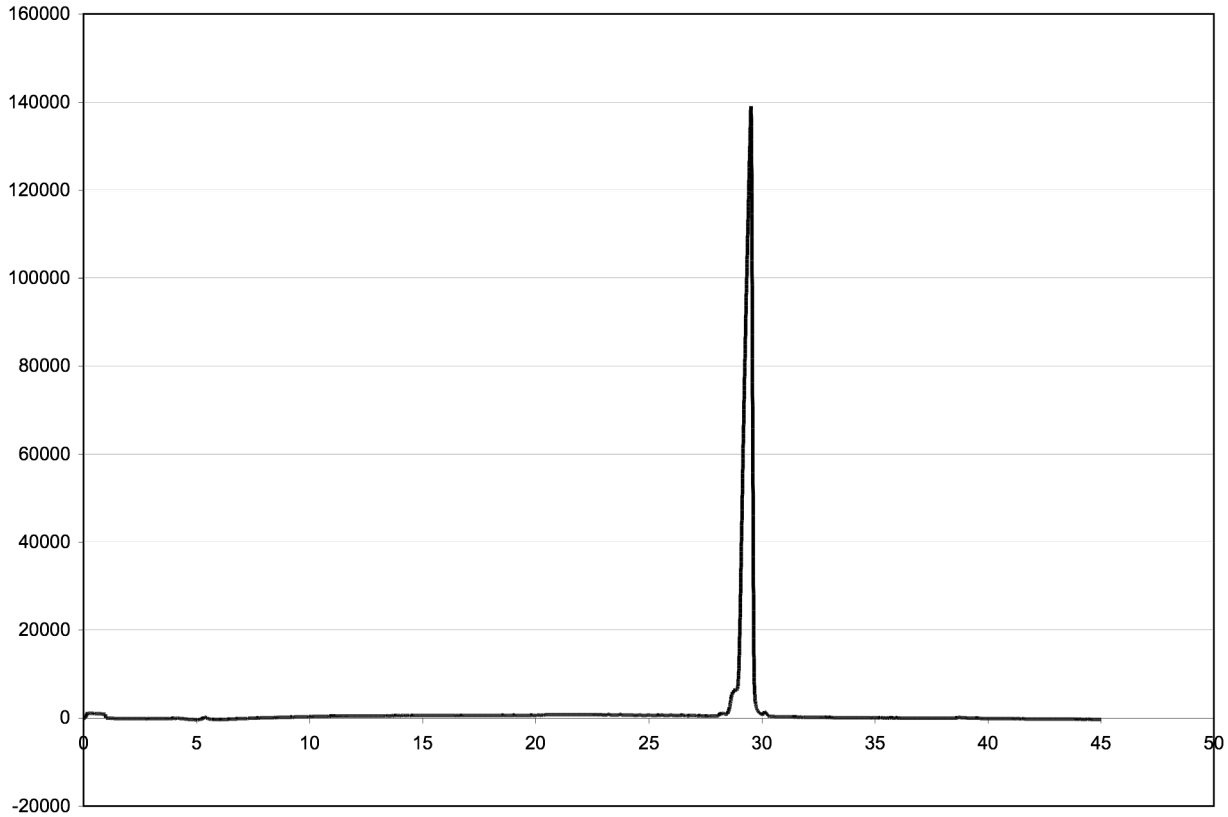

Figure S2. CGE analysis of oligonucleotide **1c**.

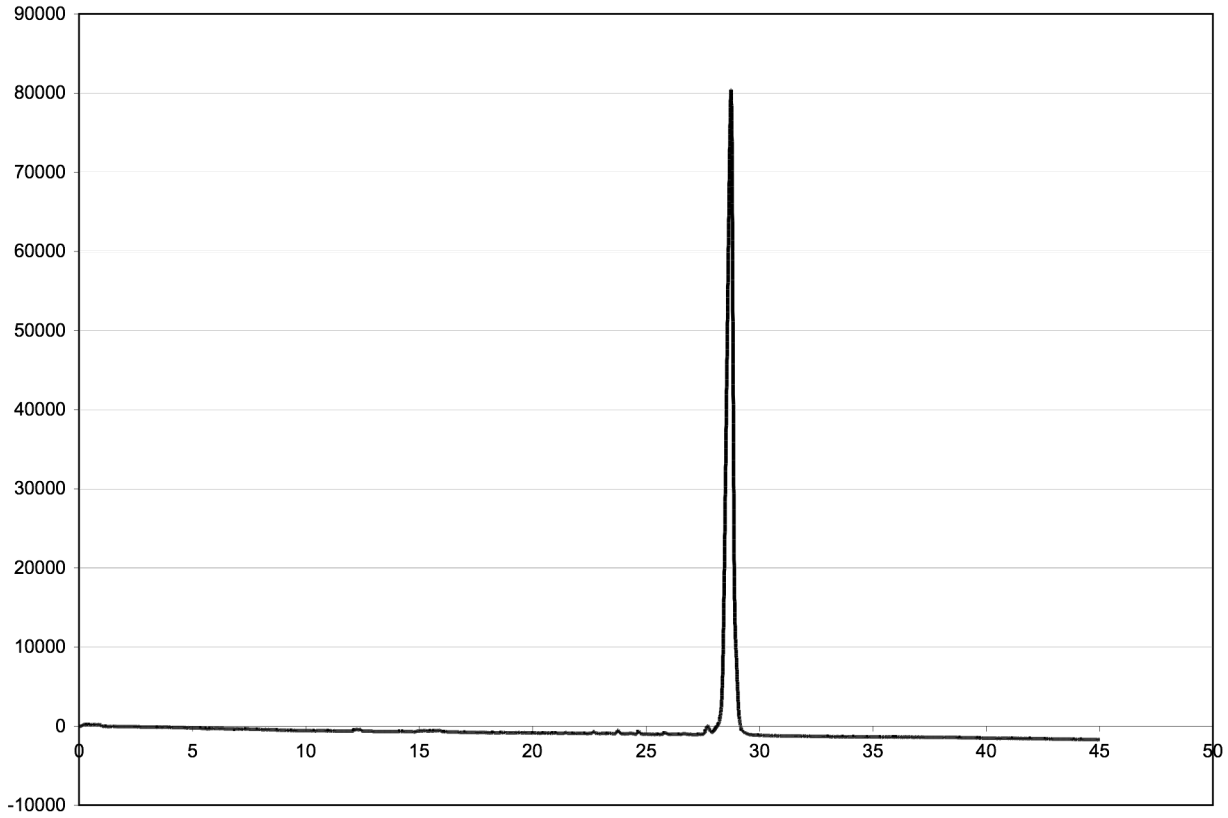

Figure S3. CGE analysis of oligonucleotide **2a**

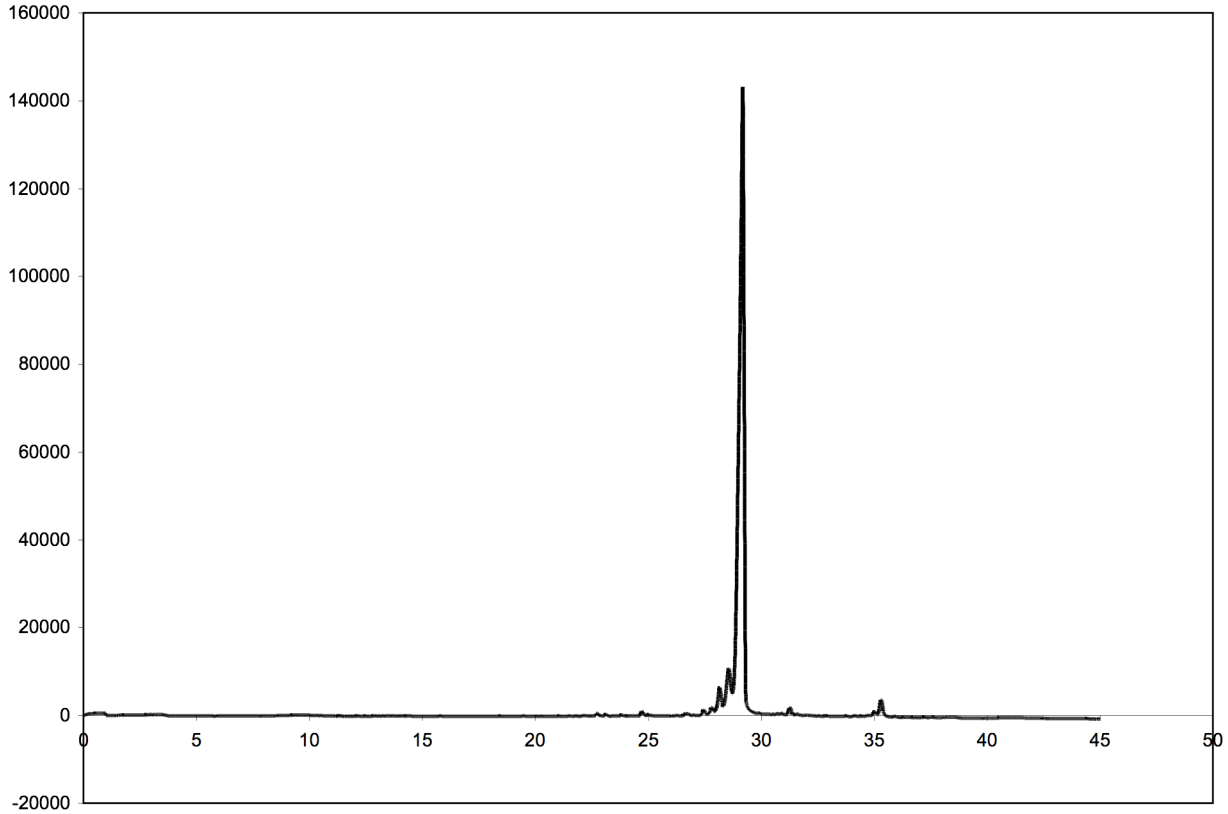

Figure S4. CGE analysis of oligonucleotide **2b**

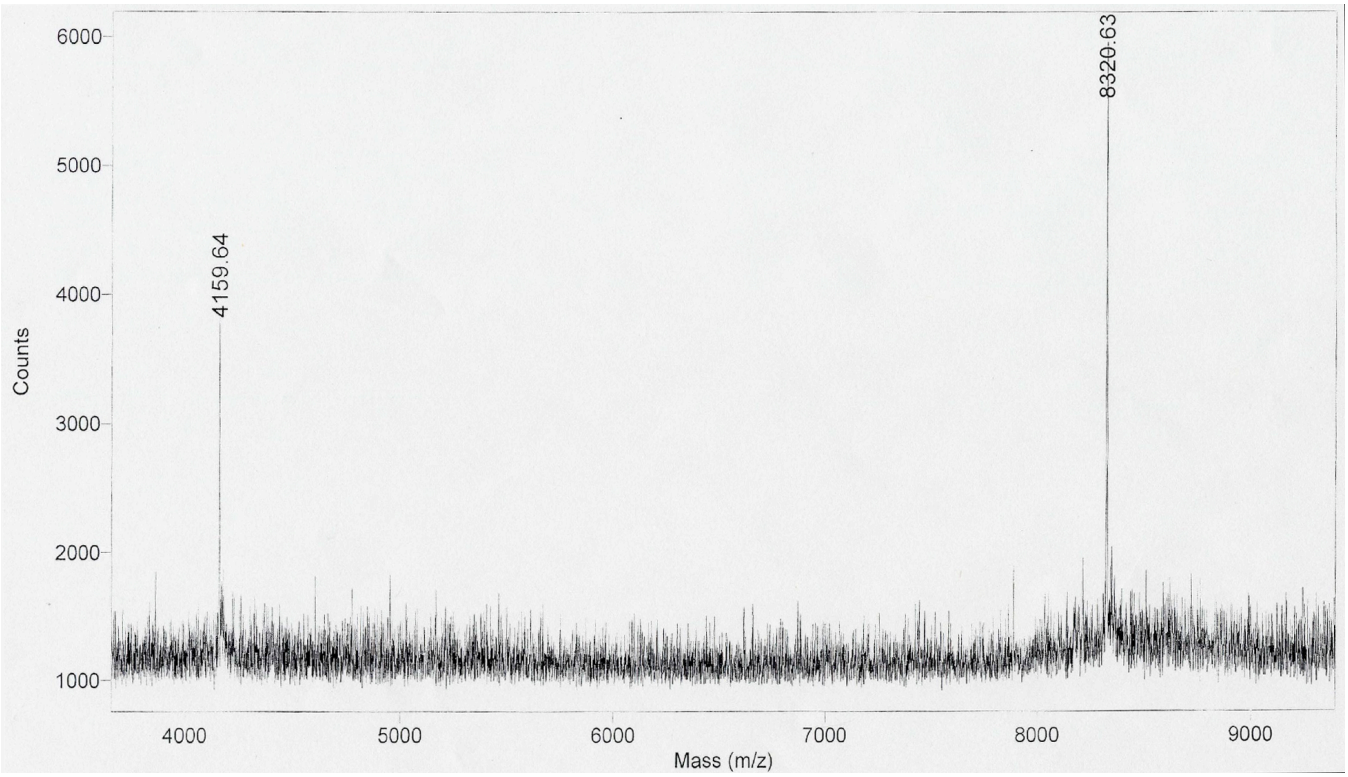

Figure S5. MALDI-TOF spectrum of oligonucleotide **1b**.

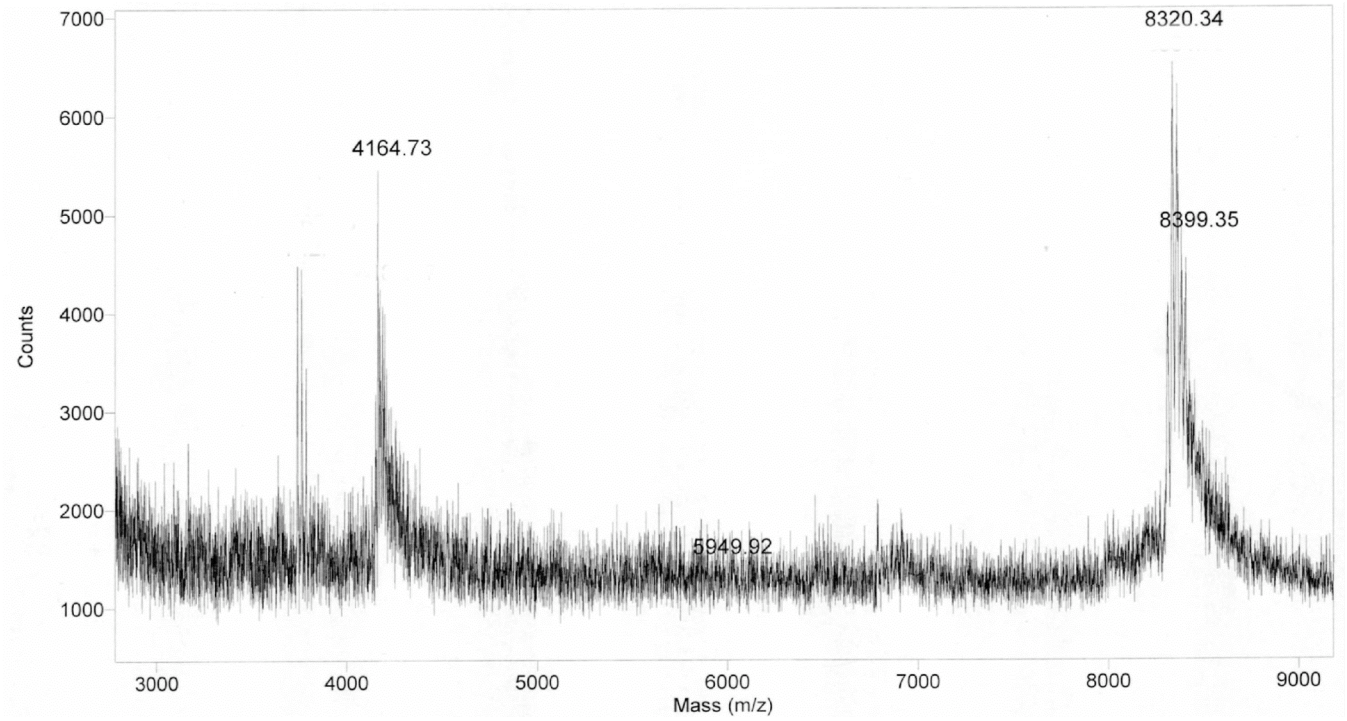

Figure S6. MALDI-TOF spectrum of oligonucleotide **1c**.

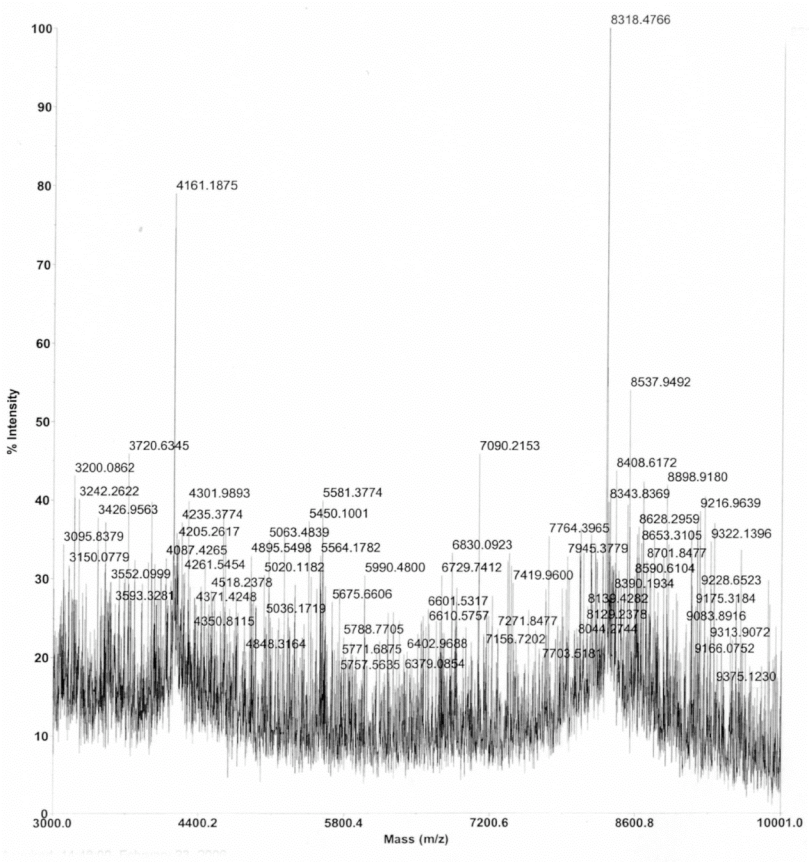

Figure S7. MALDI-TOF spectrum of oligonucleotide **2b**.

Figure S8. MALDI-TOF spectrum of oligonucleotide **2c**.

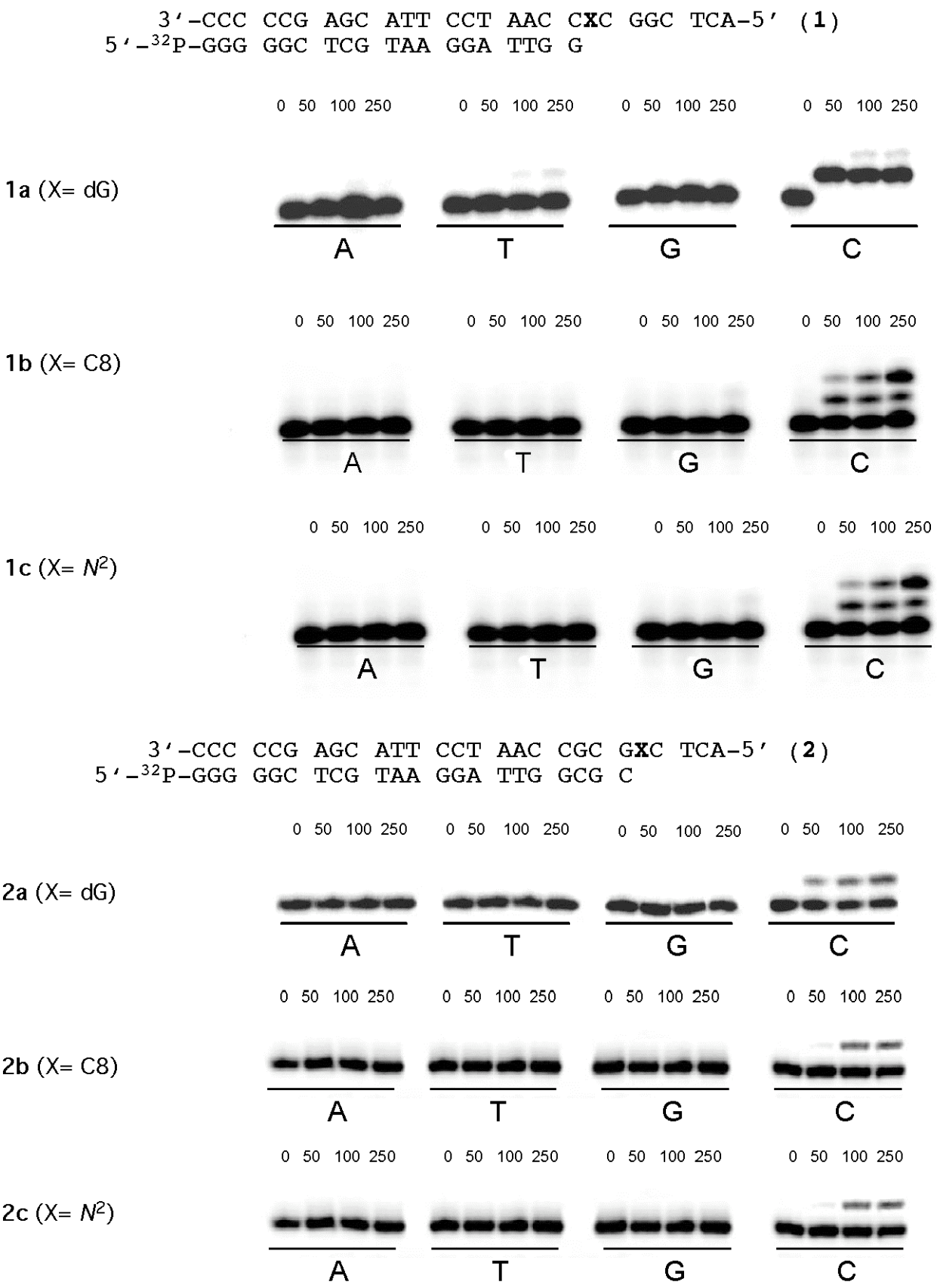

Figure S9. Single nucleotide incorporation of oligonucleotides **1a-c** and **2a-c** by Kf⁻

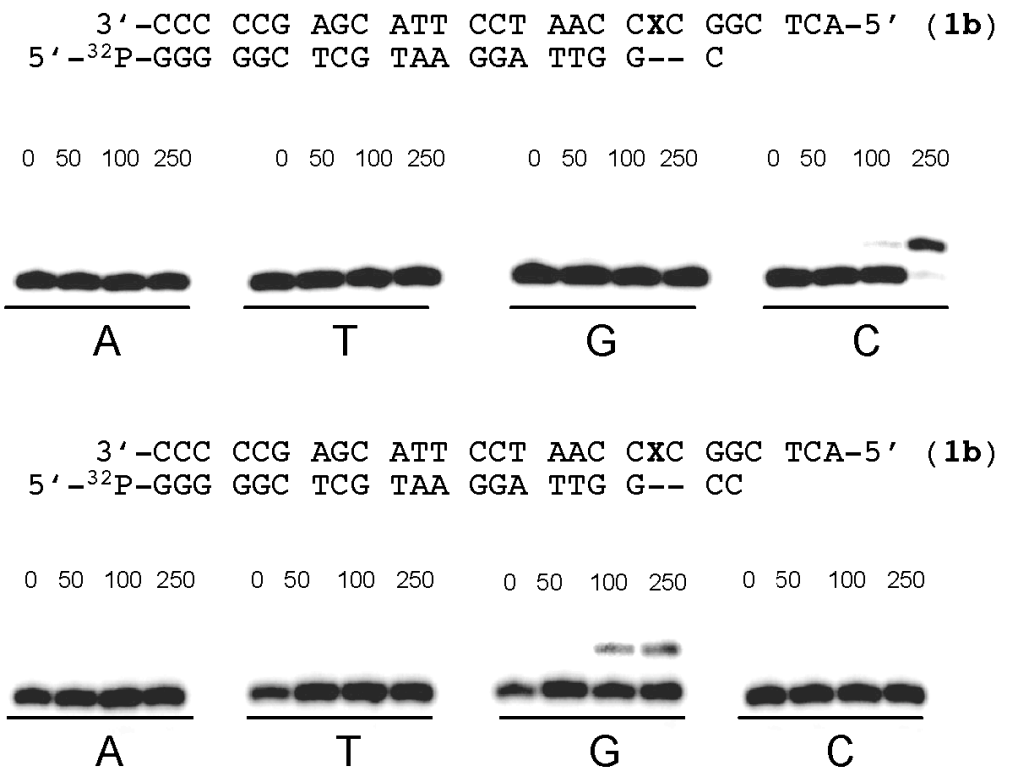

Figure S10. Single nucleotide incorporation of oligonucleotides **1b** with a 0- and +1 primers.

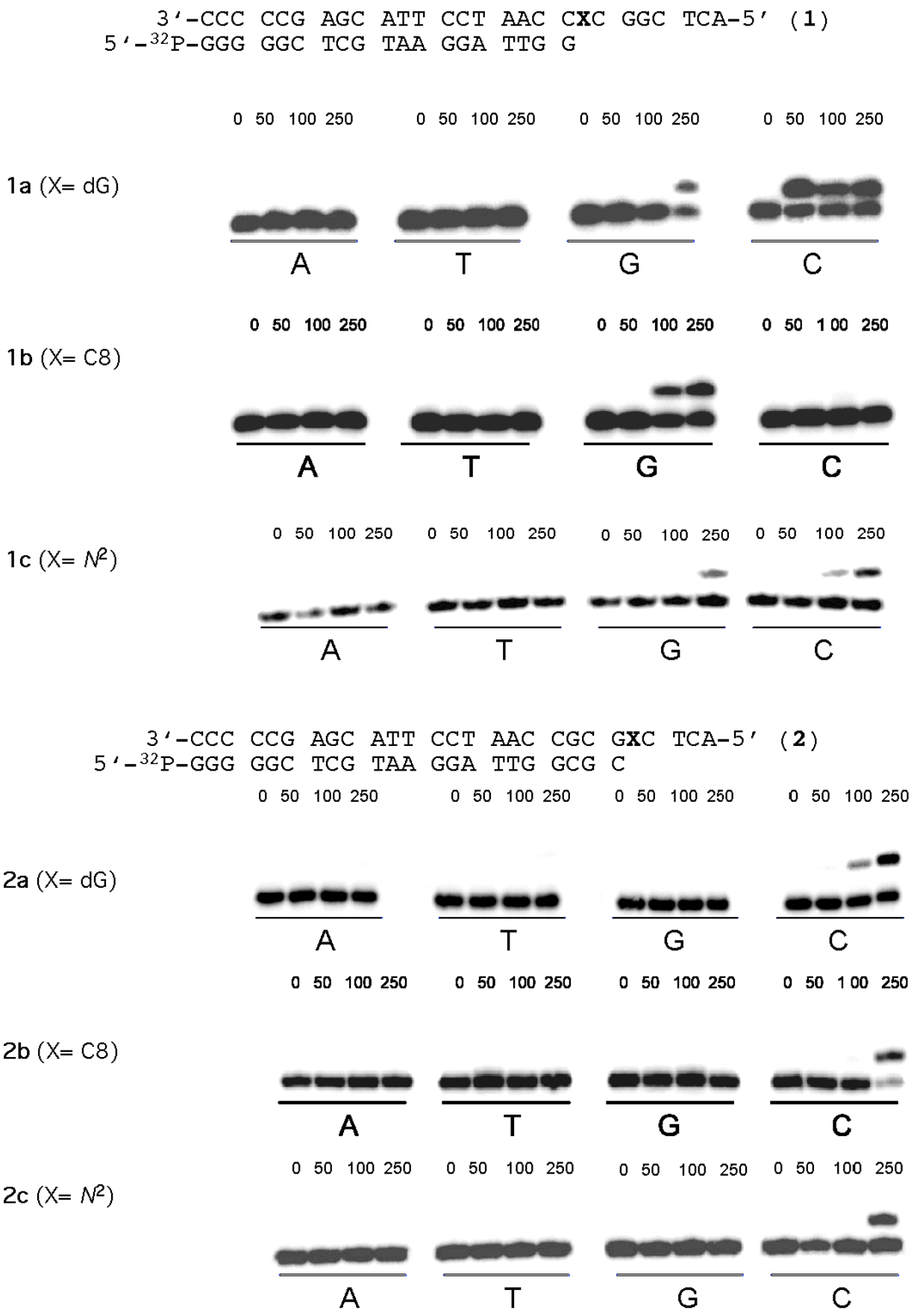

Figure S11. Single nucleotide incorporation of oligonucleotides **1a-c** and **2a-c** by pol II^{-}

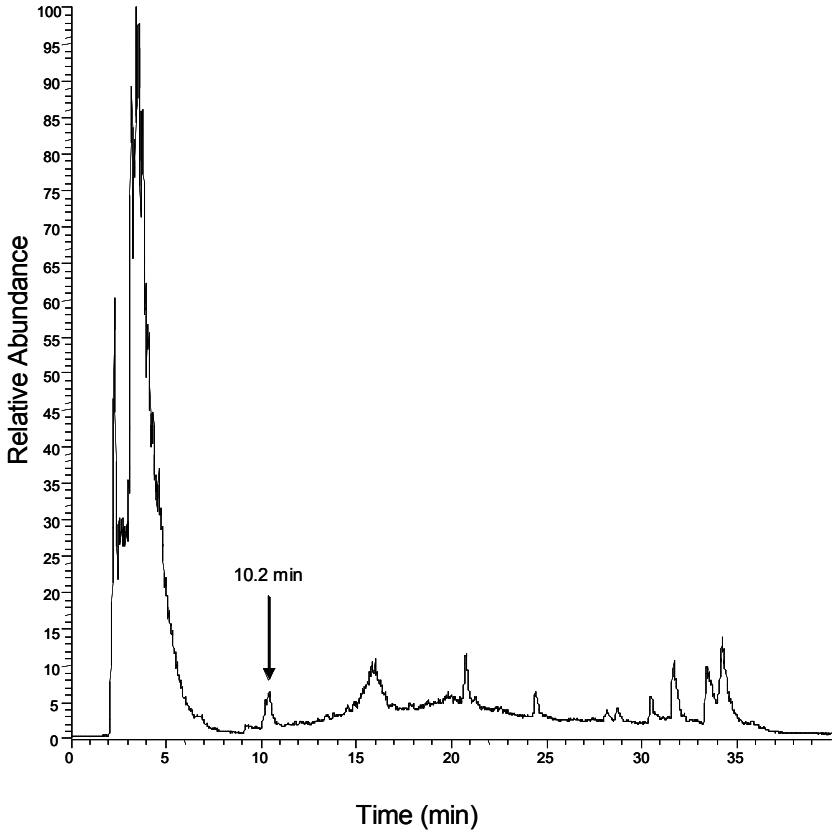

Figure S12. LC-ESI-MS/MS analysis of the pol II^{-} extension of oligonucleotide **1b**.

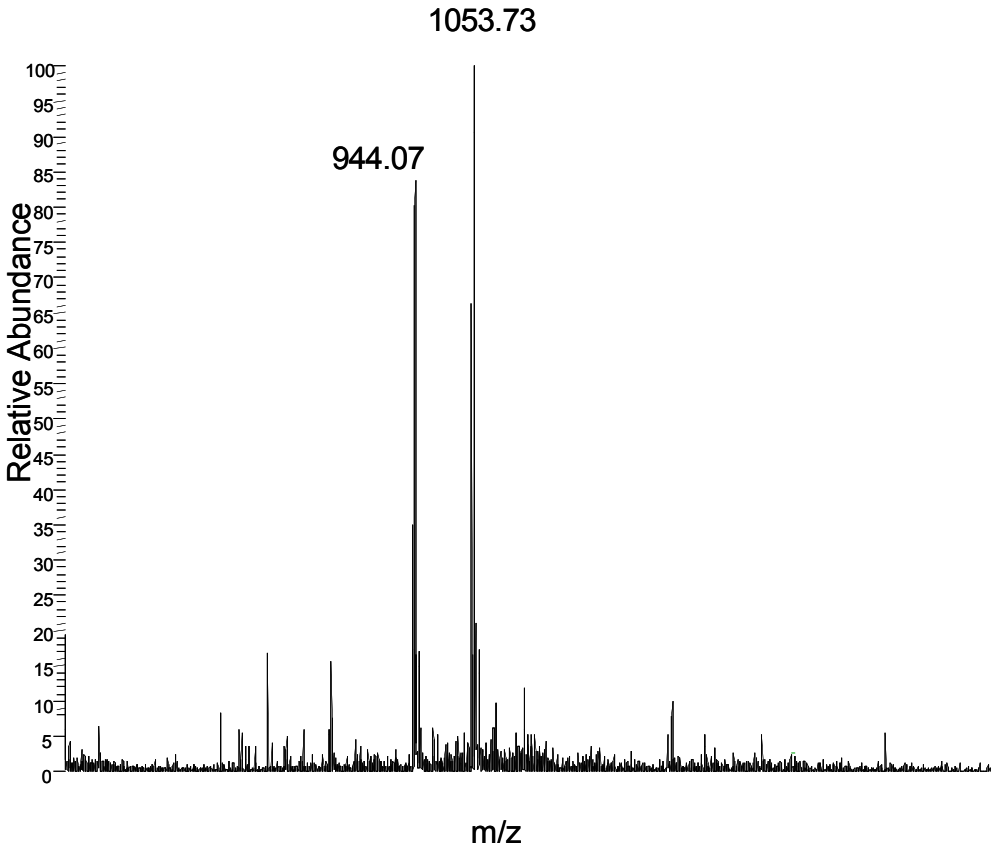

Figure S13. TIC spectrum of the pol II^{-} extension products from oligonucleotide **1b**.

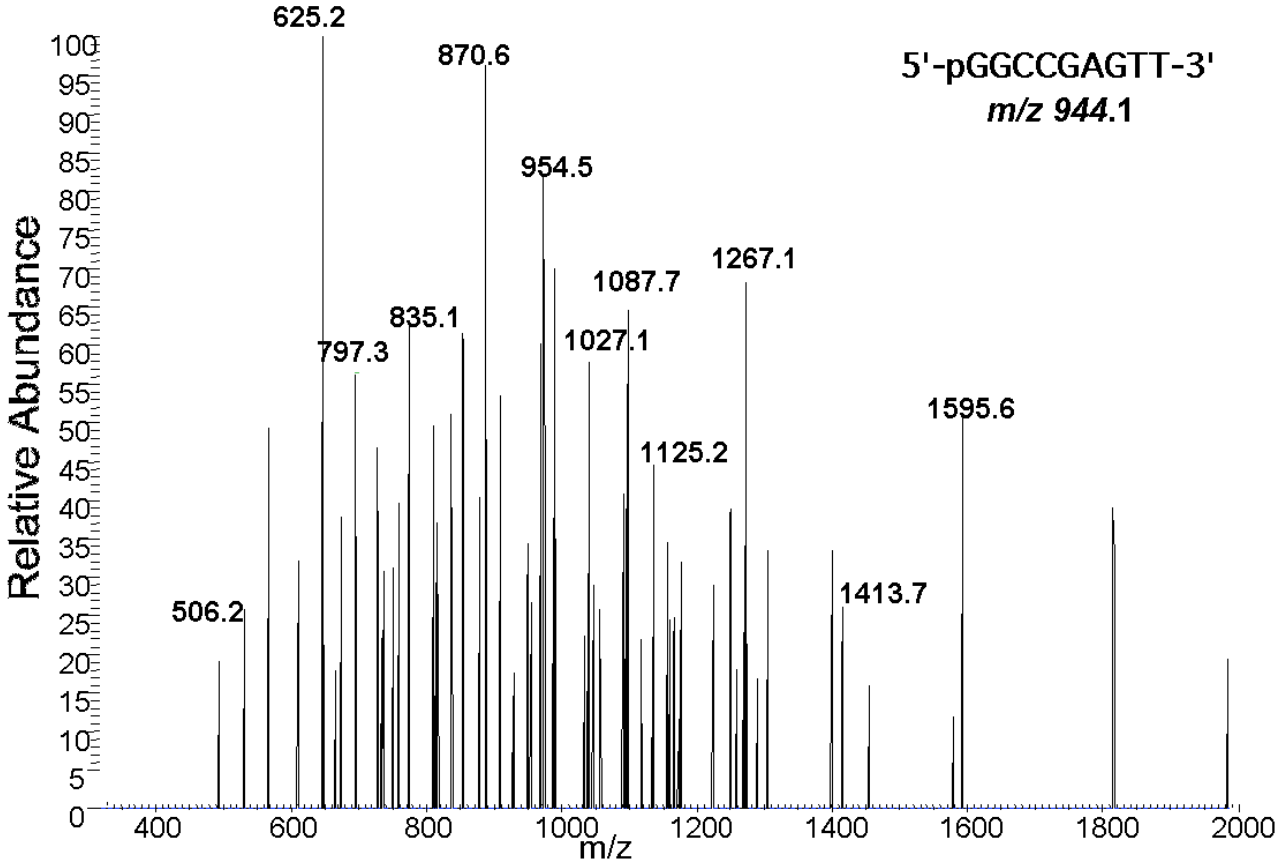

Figure S14. CID spectrum of the *m/z* 944.07 products from the pol II^{-} extension of oligonucleotide **1b**.

Table S1. Observed and calculated CID fragmentation of 5'-pGGCCGAGTT-3' (*m/z* 944.1)

Fragment assignment	observed	theoretical
5'-pG (a_2-B)	506.2	506.05
5'-pGG (a_3-B)	835.1	835.10
5'-pGGC (a_4-B)	1125.2	1124.14
5'-pGGCC (a_5-B)	1413.7	1413.19
5'-pGGCCG (a_6-B, -2)	870.7	870.62
5-pGGCCGA (a_7-B, -2)	1027.1	1027.15
pCCGAGT-3' (w_7)	1087.7	1086.67
pGAGTT-3' (w_5)	1595.6	1596.26
(w_5, -2)	797.4	797.62
pAGTT-3' (w_4)	1267.1	1267.20
pGTT-3' (w_3)	954.5	654.15
p-TT-3' (w_2)	625.3	625.09

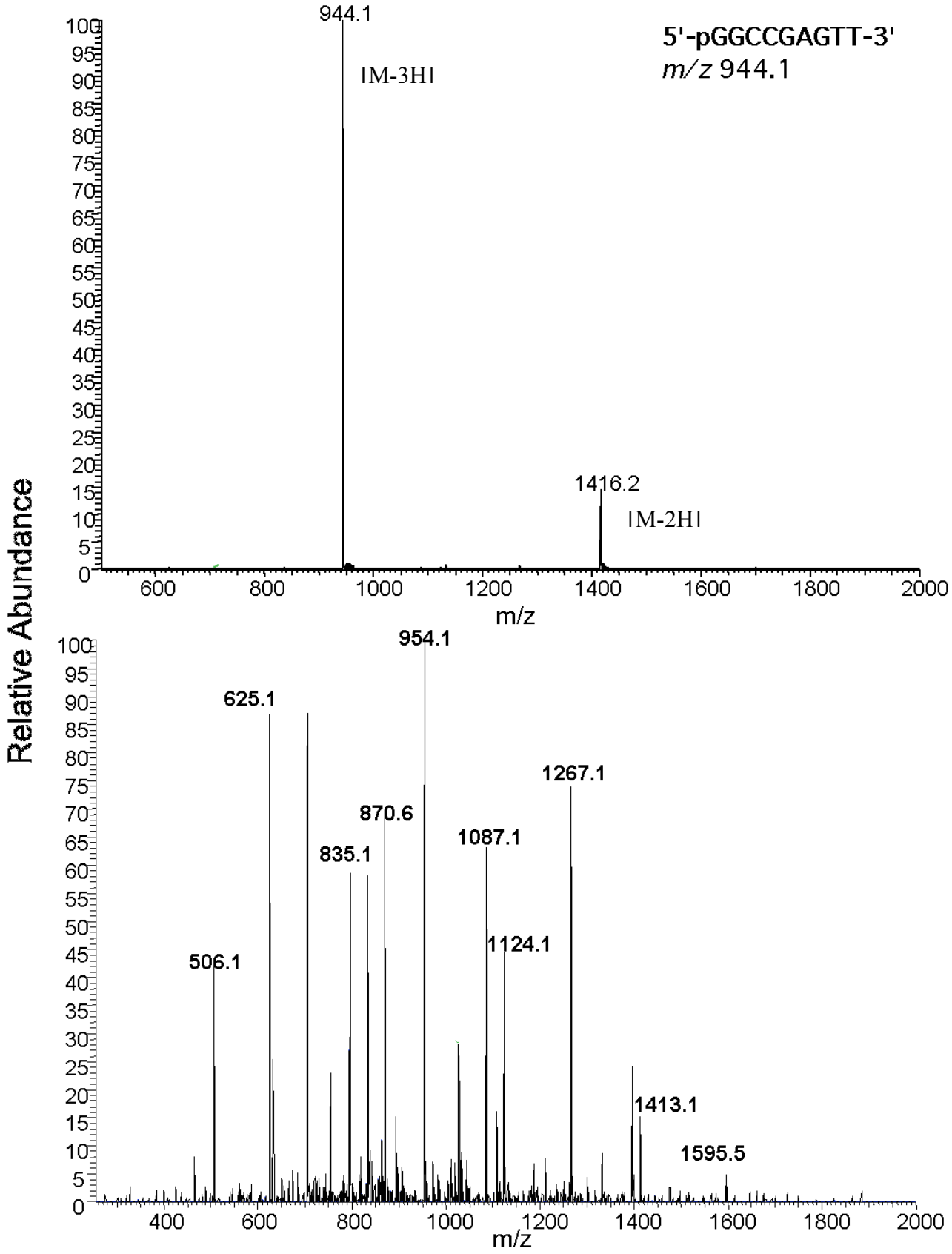

Figure S15. TIC (top) and CID (bottom) spectra of an authetic sample of 5'pGGCCGAGTT-3' (*m/z* 944.1)

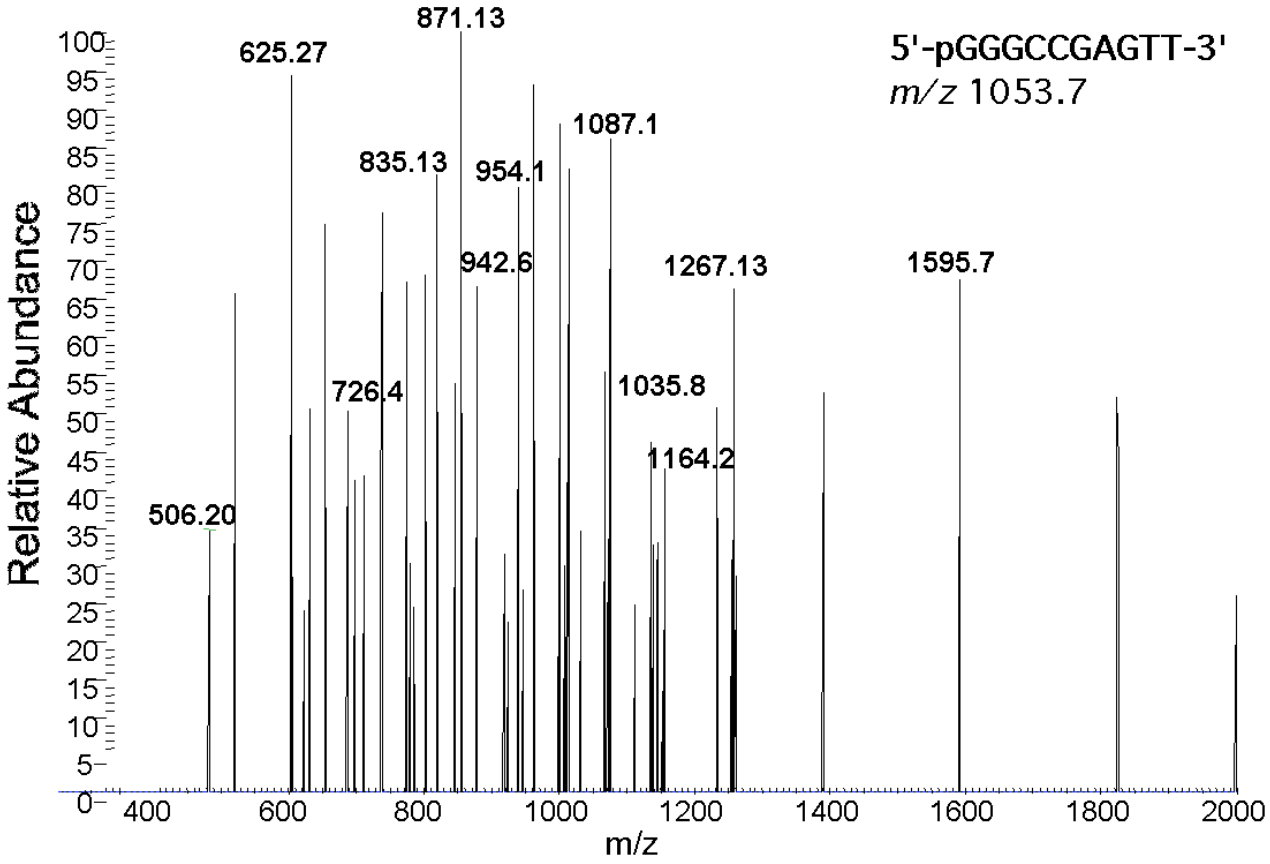

Figure S16. CID spectrum of the *m/z* 1053.7 products from the pol II⁻ extension of oligonucleotide **1b**.

Table S2. Observed and calculated CID fragmentation of 5'-pGGGCCGAGTT-3' (*m/z* 1053.7)

Fragment assignment	observed	theoretical
5'-pG (a_2-B)	506.2	506.05
5'-pGG (a_3-B)	835.1	835.10
5'-pGGG (a_4-B)	1164.2	1164.15
5'-pGGGC (a_5-B, -2)	726.4	726.09
5'-pGGGCC (a_6-B, -2)	871.13	870.62
5-pGGGCCG (a_7-B, -2)	1035.8	1035.14
pCCGAGTT-3' (w_7, -2)	1087.1	1086.67
pCCGAGTT-3' (w_6, -2)	942.6	942.15
pGAGTT-3' (w_5)	1595.7	1596.26
pAGTT-3' (w_4)	1267.1	1267.20
pGTT-3' (w_3)	954.5	954.15
p-TT-3' (w_2)	625.3	625.09

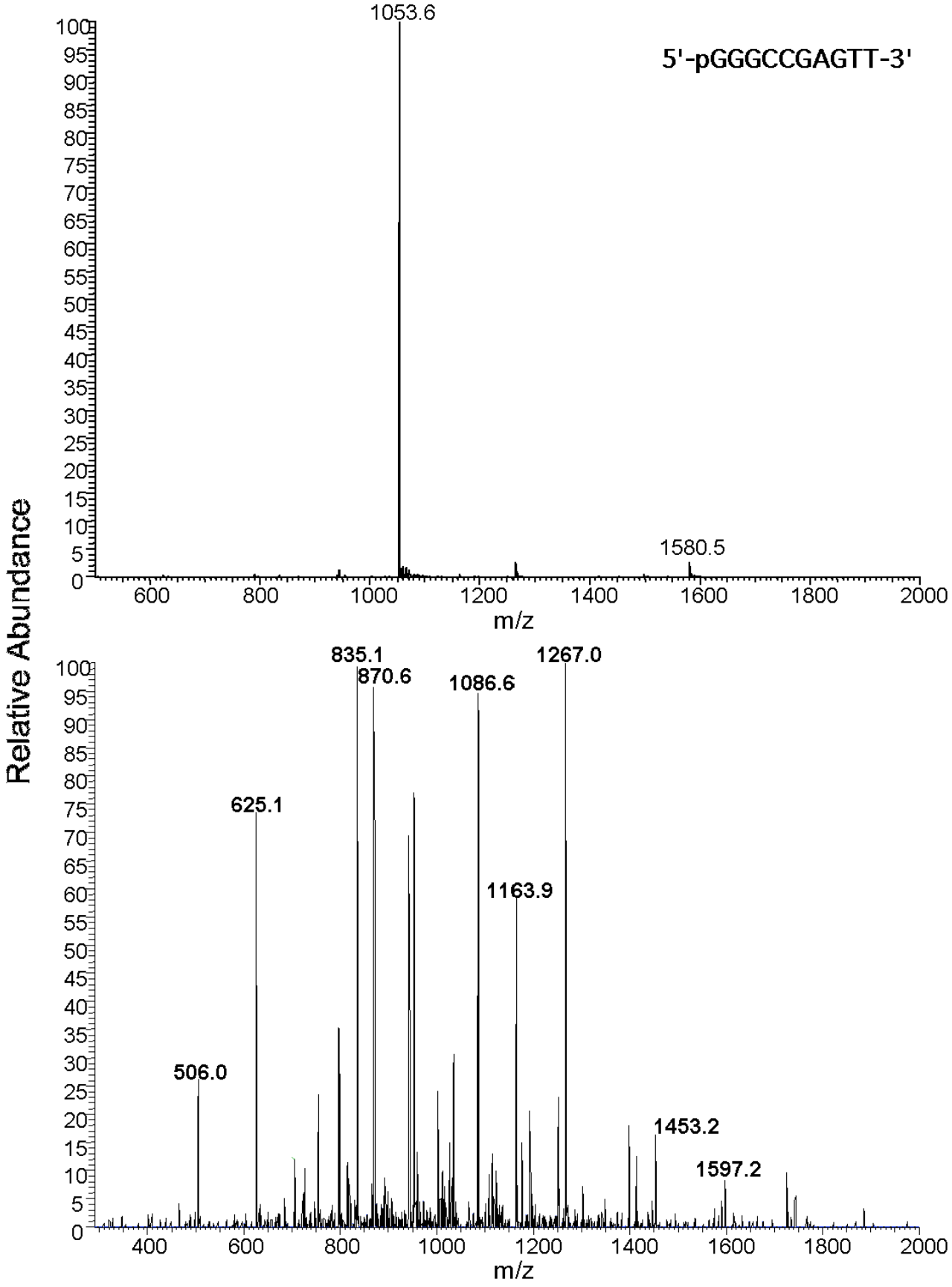

Figure S17. TIC (top) and CID (bottom) spectra of an authentic sample of 5'pGGGCCGAGTT-3' (*m/z* 1053.7)

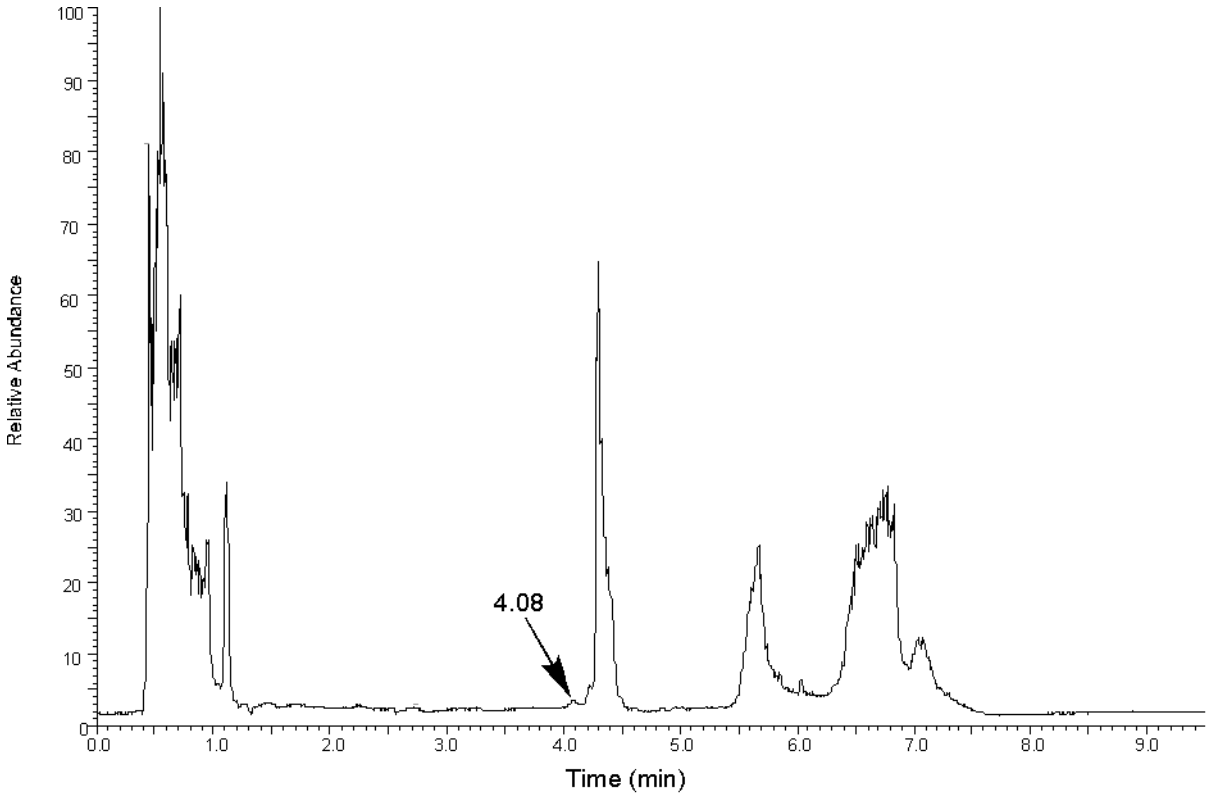

Figure S18. LC-ESI-MS/MS analysis of the pol II^{-} extension of oligonucleotide **2b**

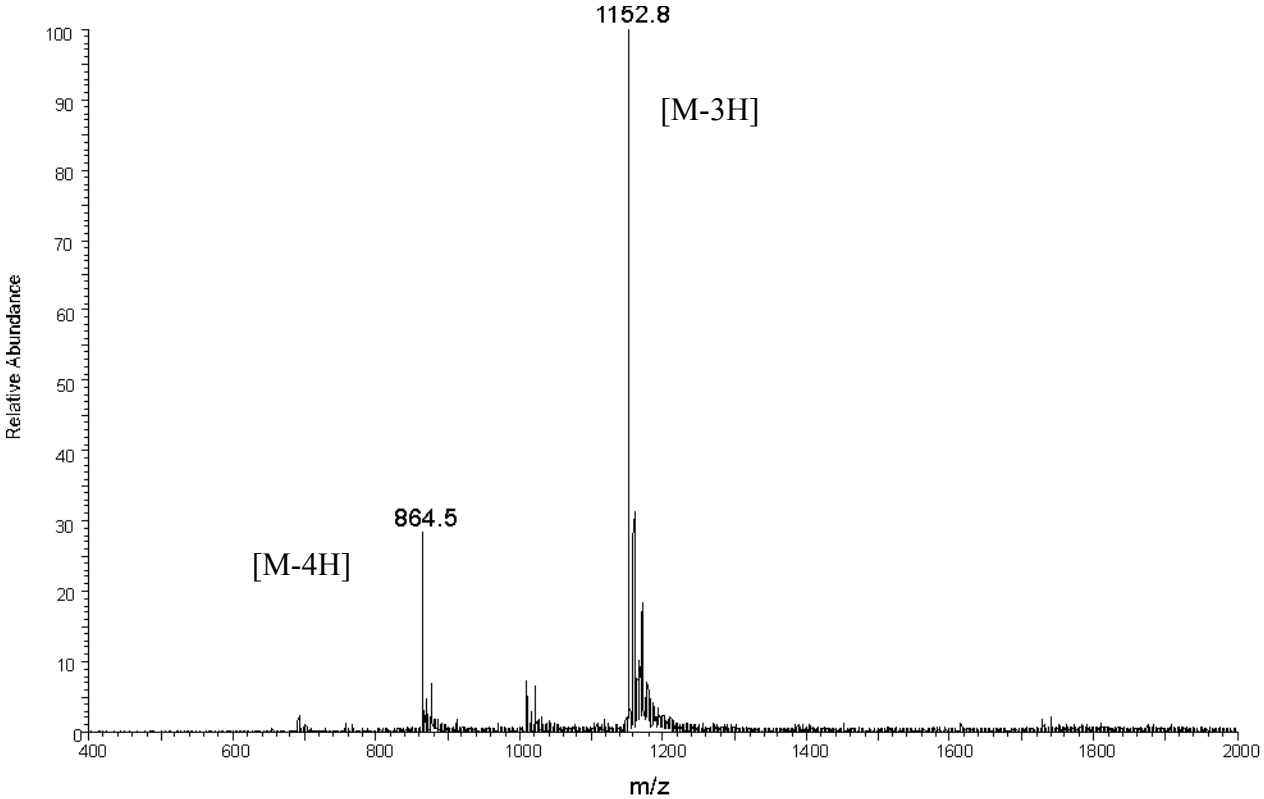

Figure S19. TIC spectrum of the pol II^{-} extension products from oligonucleotide **2b**

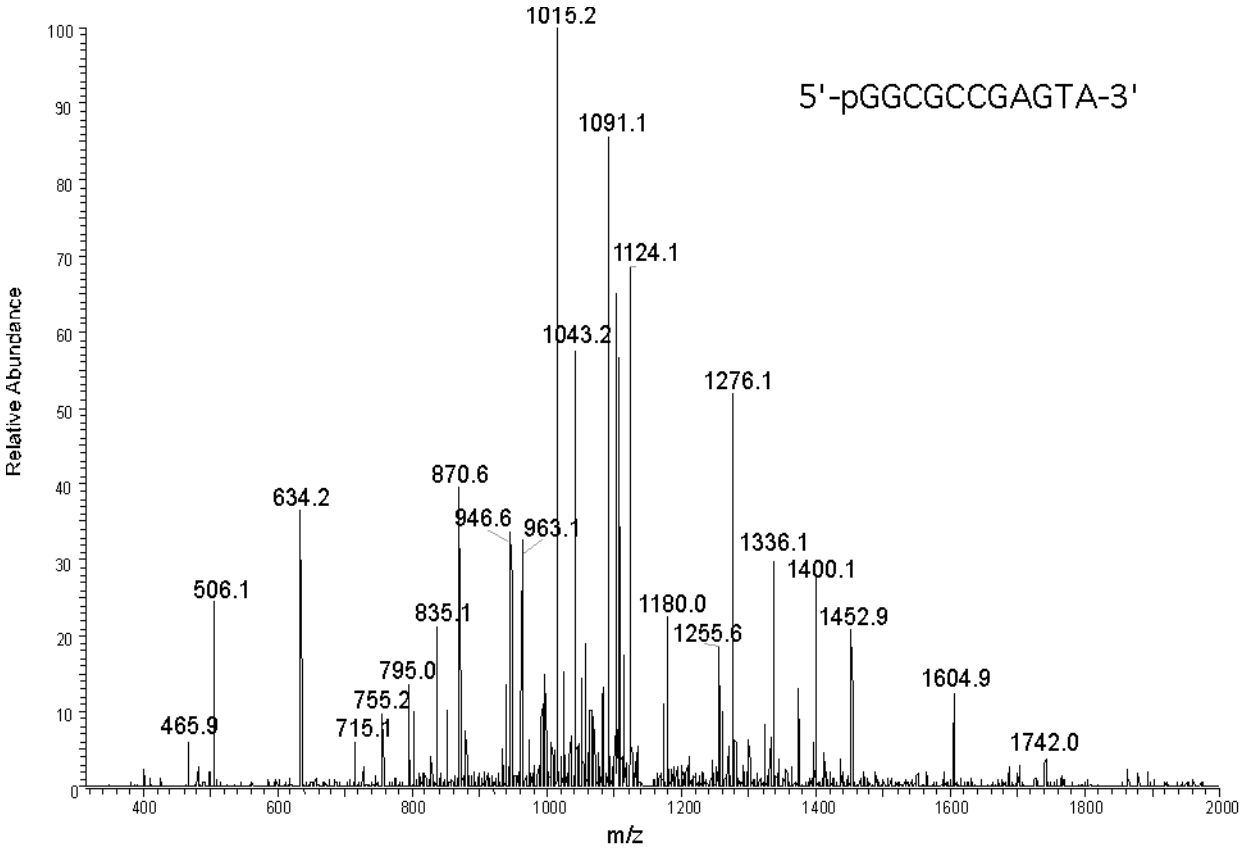

Figure S20. CID spectrum of the *m/z* 1152.8 products from the pol II⁻ extension of oligonucleotide **2b**.

Table S3. Observed and calculated CID fragmentation of 5'-pGGCGCCGAGTA-3' (*m/z* 10152.8)

Fragment assignment	observed	theoretical
5'-pG (a_2-B)	506.1	506.05
5'-pGG (a_3-B)	835.1	835.10
5'-pGGC (a_4-B)	1124.1	1124.14
5'-pGGCG (a_5-B)	1452.9	1453.20
5'-pGGCGC (a_6-B)	1742.0	1742.2
(a_6-B, -2)	870.6	870.62
5-pGGCGCC (a_7-B, -2)	1015.2	1015.14
5-pGGCGCCG (a_8-B, -2)	1180.0	1179.67
5-pGGCGCCG (a_9-B, -2)	1336.1	1336.20
pCGCCGAGTA-3' (w_9, -2)	1400.1	1400.22
pGCCGAGTA-3' (w_8, -2)	1255.9	1255.70
pCCGAGTA-3' (w_7, -2)	1091.2	1091.18
pCGAGTA-3' (w_6, -2)	946.6	946.65
pGAGTA-3' (w_5)	1604.9	1605.27
pAGTA-3' (w_4)	1276.1	1276.21
pGTA-3' (w_3)	963.1	963.16
p-TA-3' (w_2)	634.2	634.11

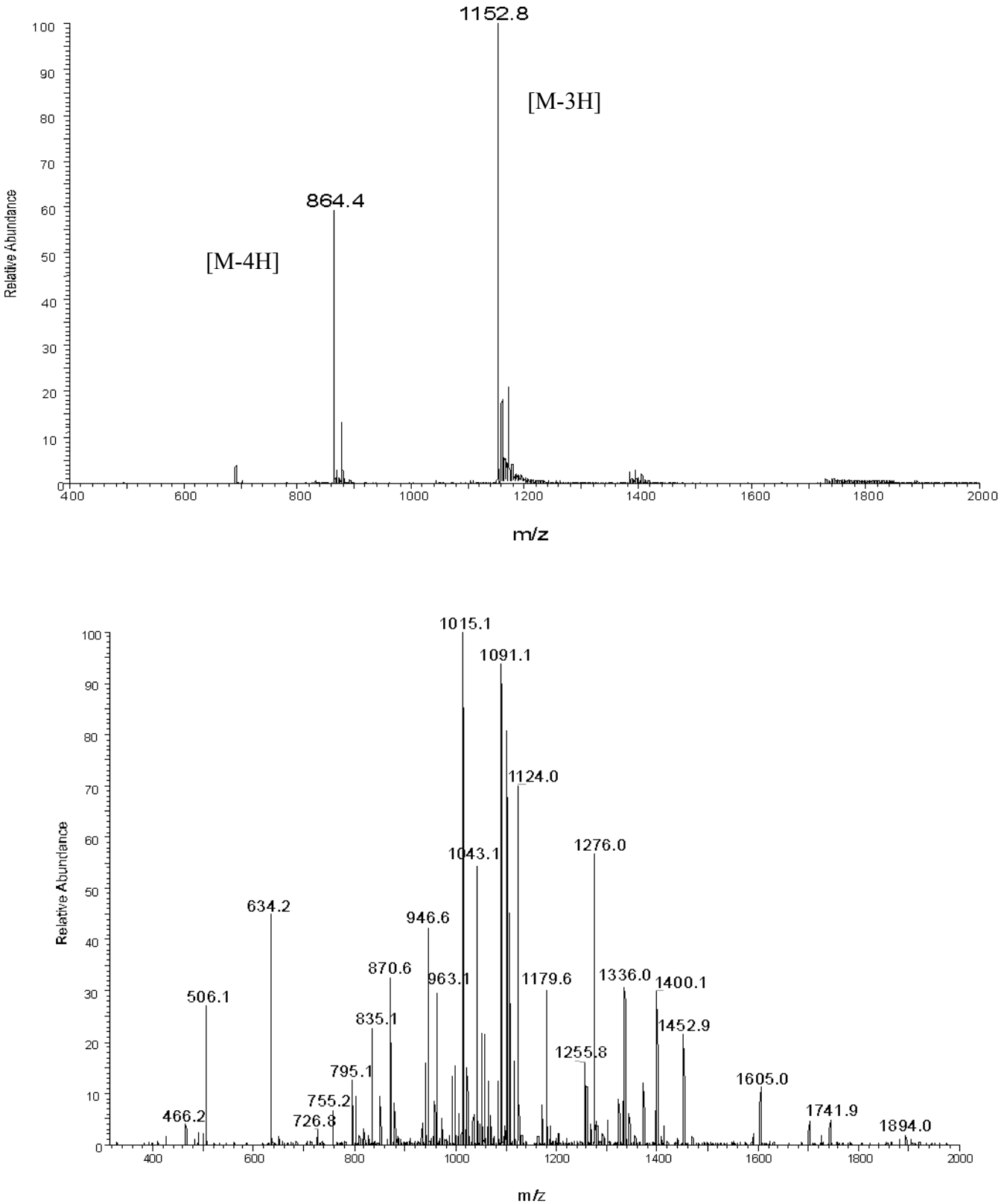

Figure S21. TIC (top) and CID (bottom) spectra of an authentic sample of 5'pGGCGCCGAGTA-3' (*m/z* 1052)

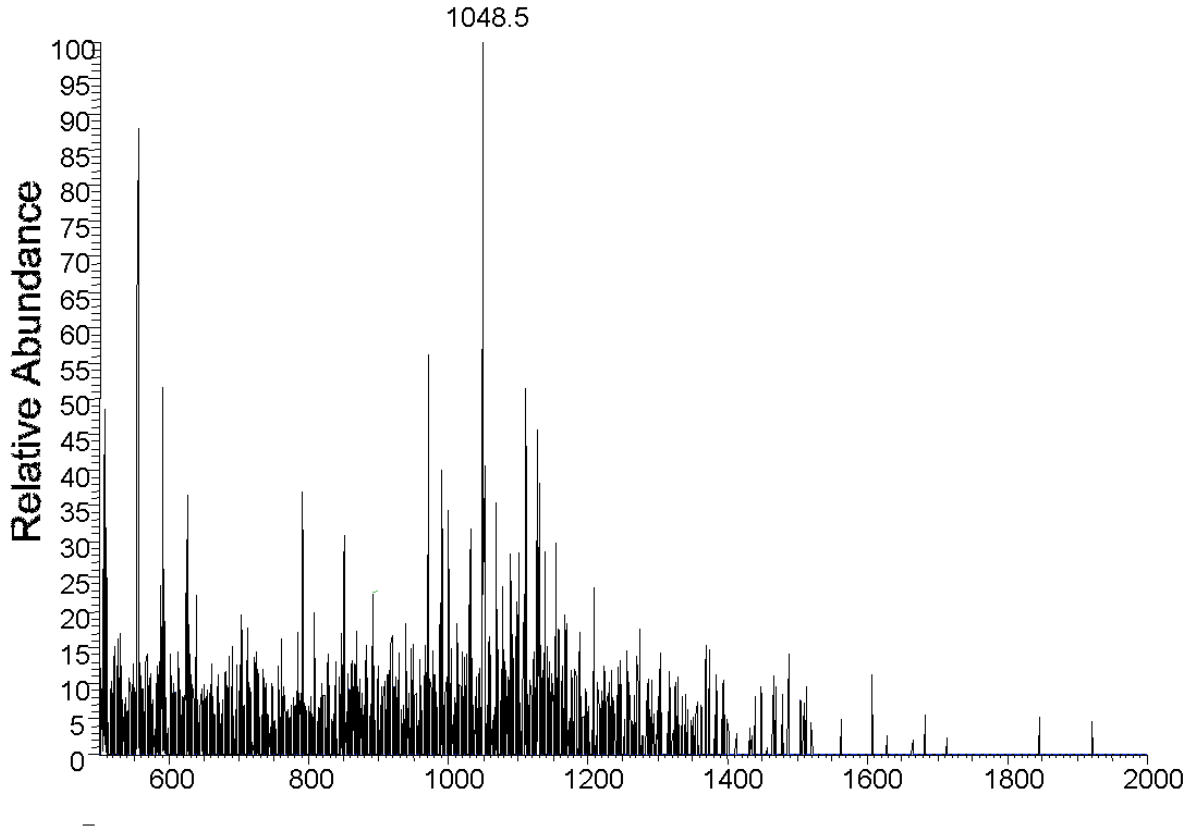

Figure S22. TIC spectrum of the pol II⁻ extension of oligonucleotide **2c**

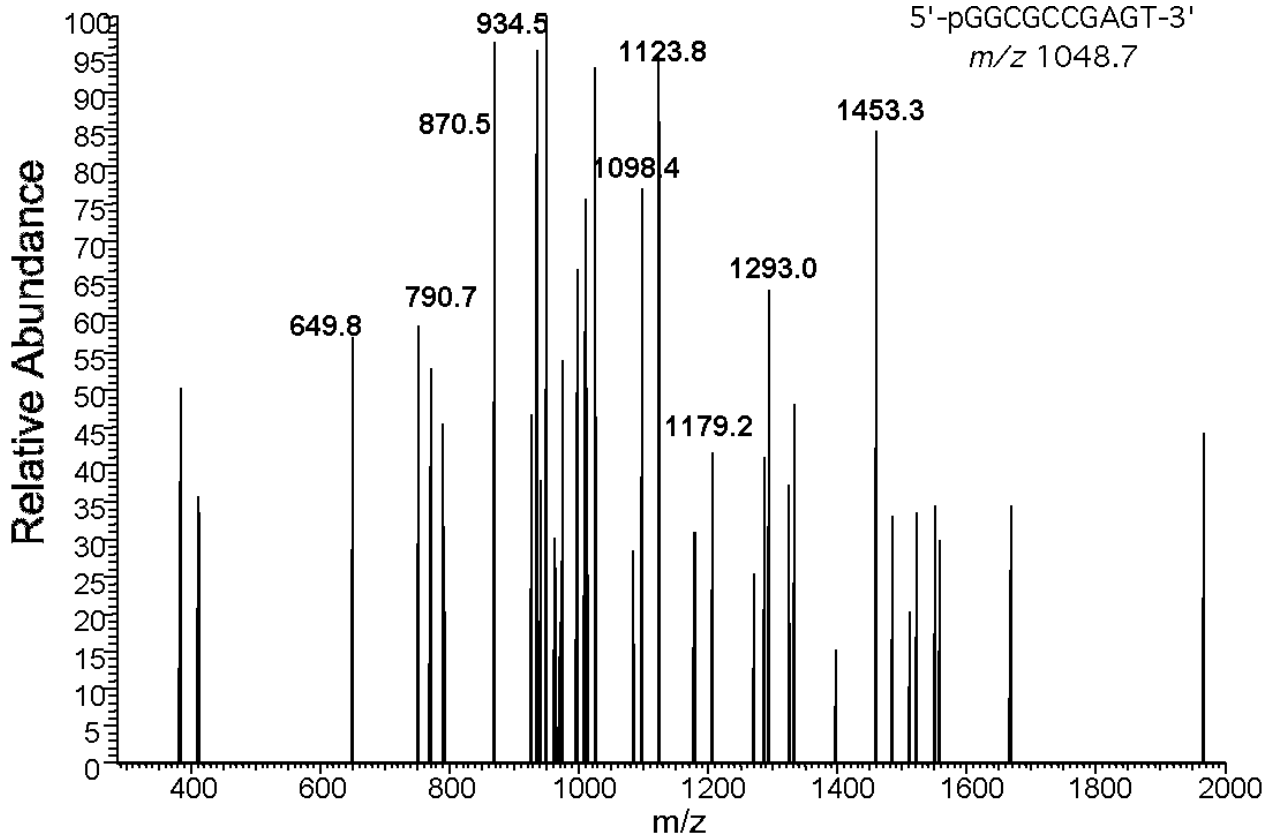

Figure S23. CID spectrum of the *m/z* 1048.7 product from the pol II⁻ extension of oligonucleotide **2c**.

Table S4. Observed and calculated CID fragmentation of 5'-pGGCGCCGAGT-3'; *m/z* 1048.7 (M-3H)

Fragment assignment	observed	theoretical
5'-pGGC (a_4-B)	1124.0	1124.14
5'-pGGCG (a_5-B)	1453.0	1453.20
5'-pGGCGC (a_6-B, -2)	870.5	870.62
5'-pGGCGCCG (a_8-B, -2)	1179.2	1179.67
pGCCGAGT-3' (w_7, -2)	1098.4	1099.17
pCCGAGT-3' (w_6, -2)	934.5	934.65
pCGAGT-3' (w_5, -2)	790.7	790.12
pGAGT-3' (w_4)	1293.0	1292.21
pAGT-3' (w_3)	963.2	963.16
pGT-3' (w_2)	649.8	650.10

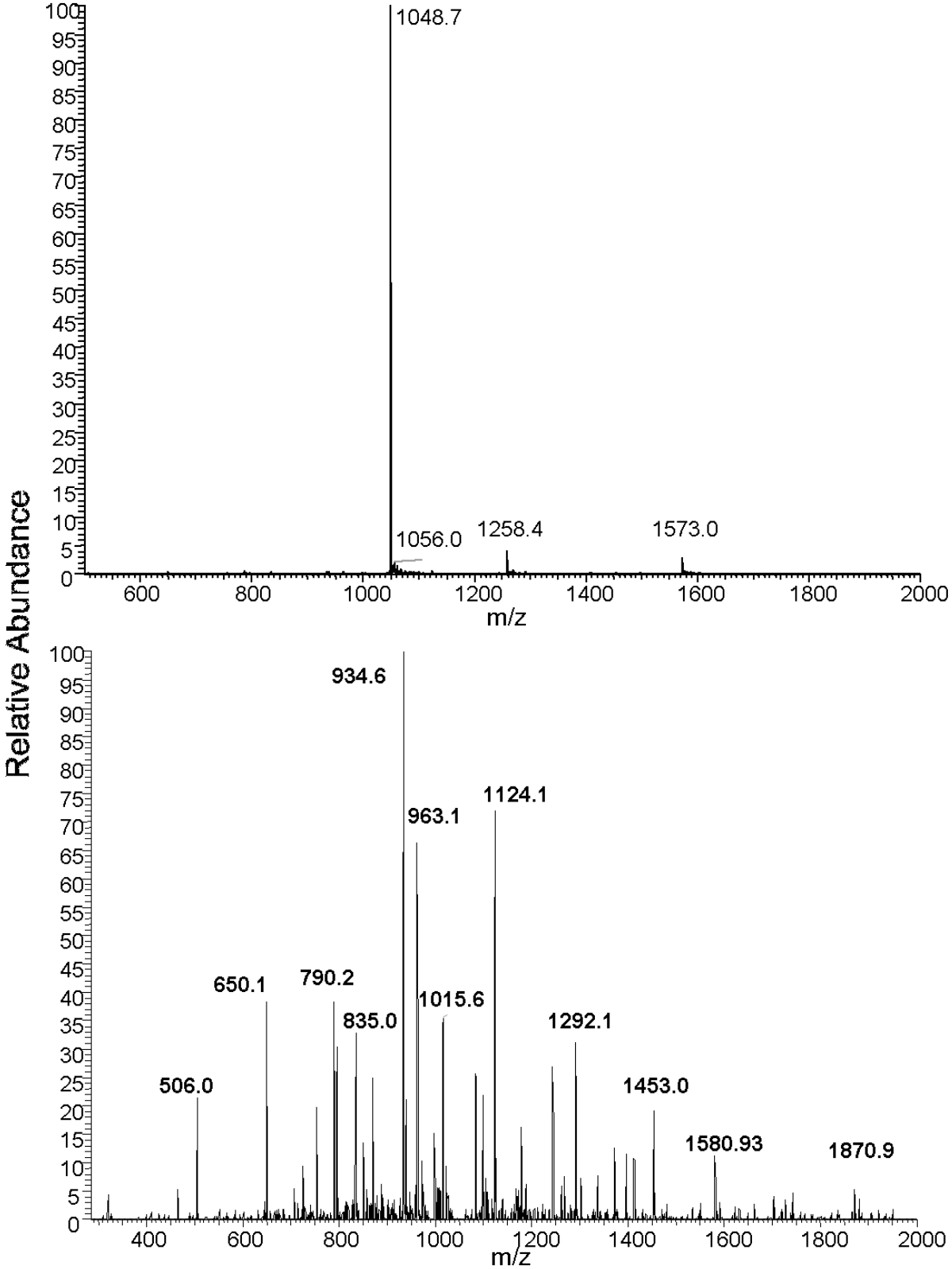

Figure S24. TIC (top) and CID (bottom) spectra of an authentic sample of 5'pGGCGCCGAGT-3' (*m/z* 1048.7)

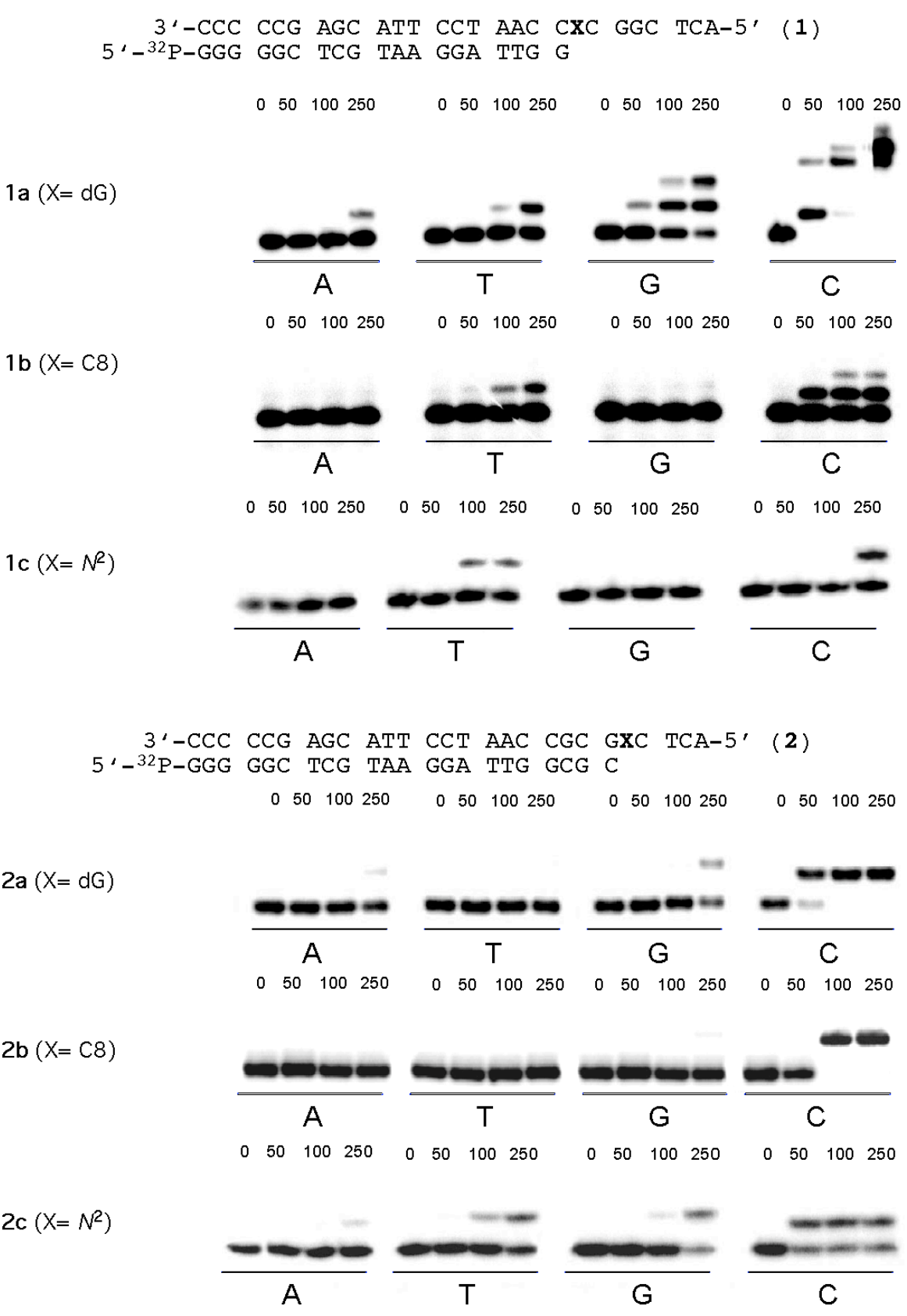

Figure S25. Single nucleotide incorporation of oligonucleotides **1a-c** and **2a-c** by Dpo4

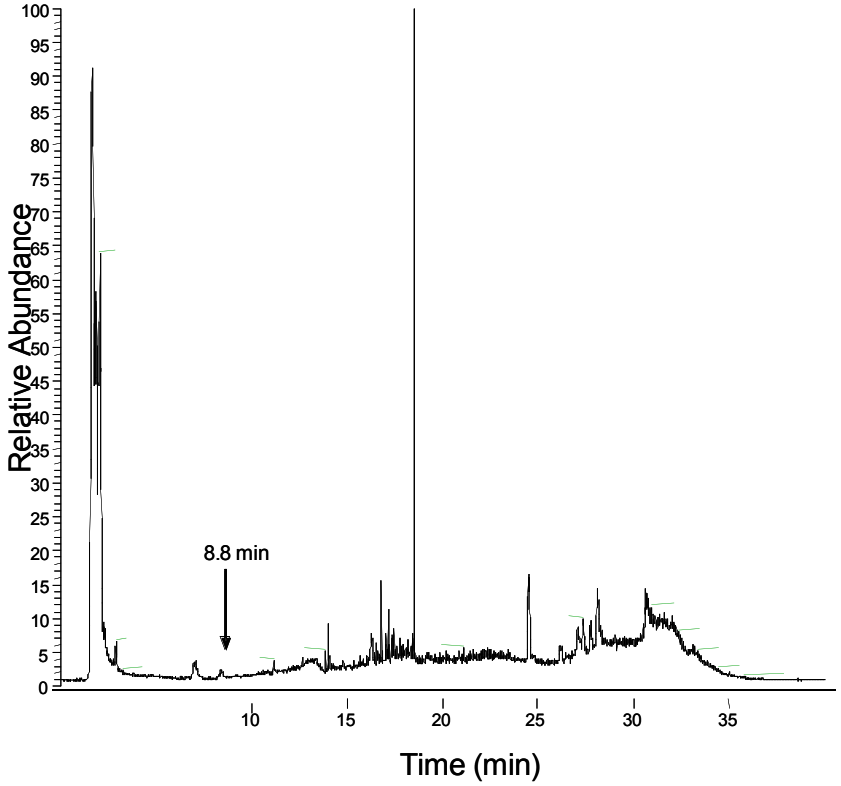

Figure S26. LC-ESI-MS/MS analysis of the Dpo4 extension of oligonucleotide **1b**.

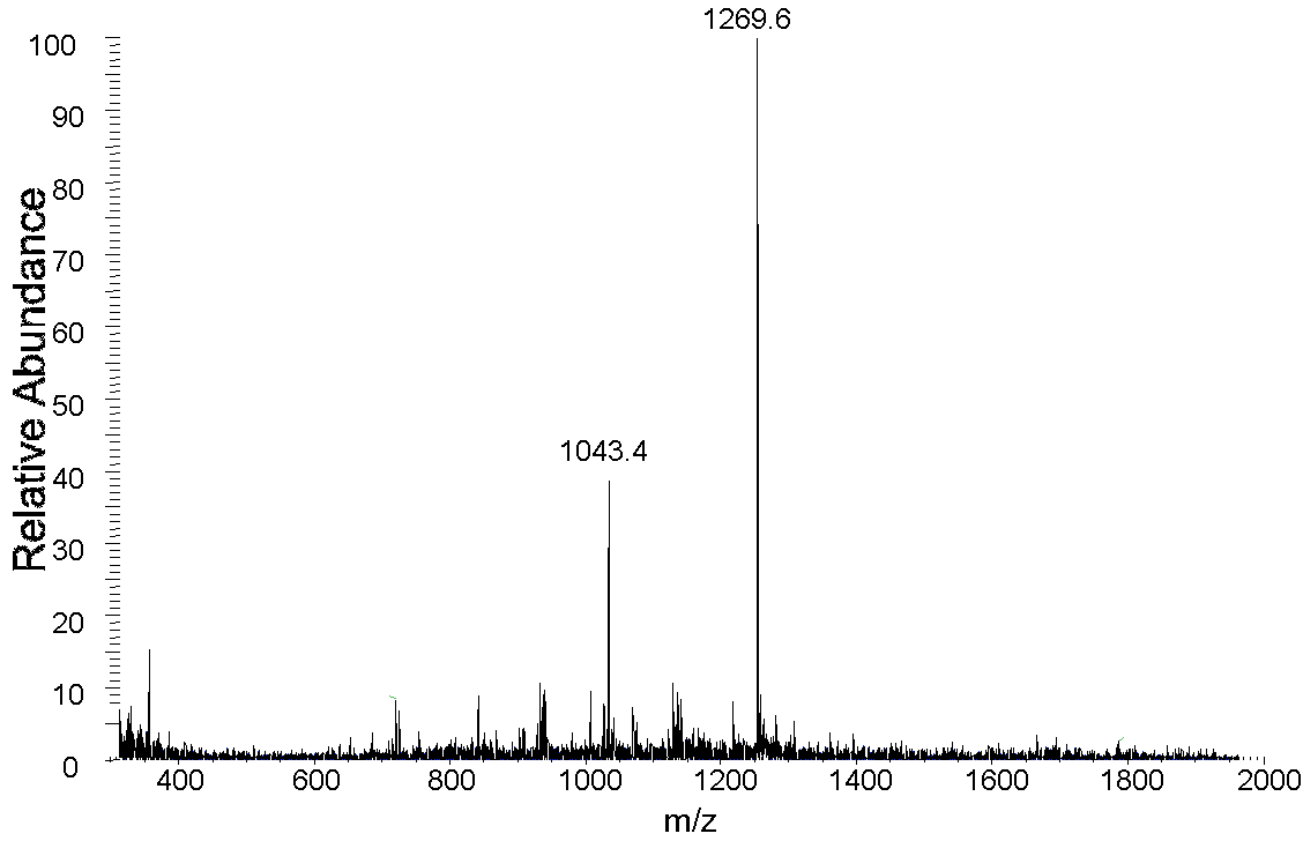

Figure S27. TIC spectrum of the Dpo4 extension products from oligonucleotide **1b**. The m/z 1269.6 is from the 5'-end of the primer (5'-GGGGGCTCGTAAGGATp-3')

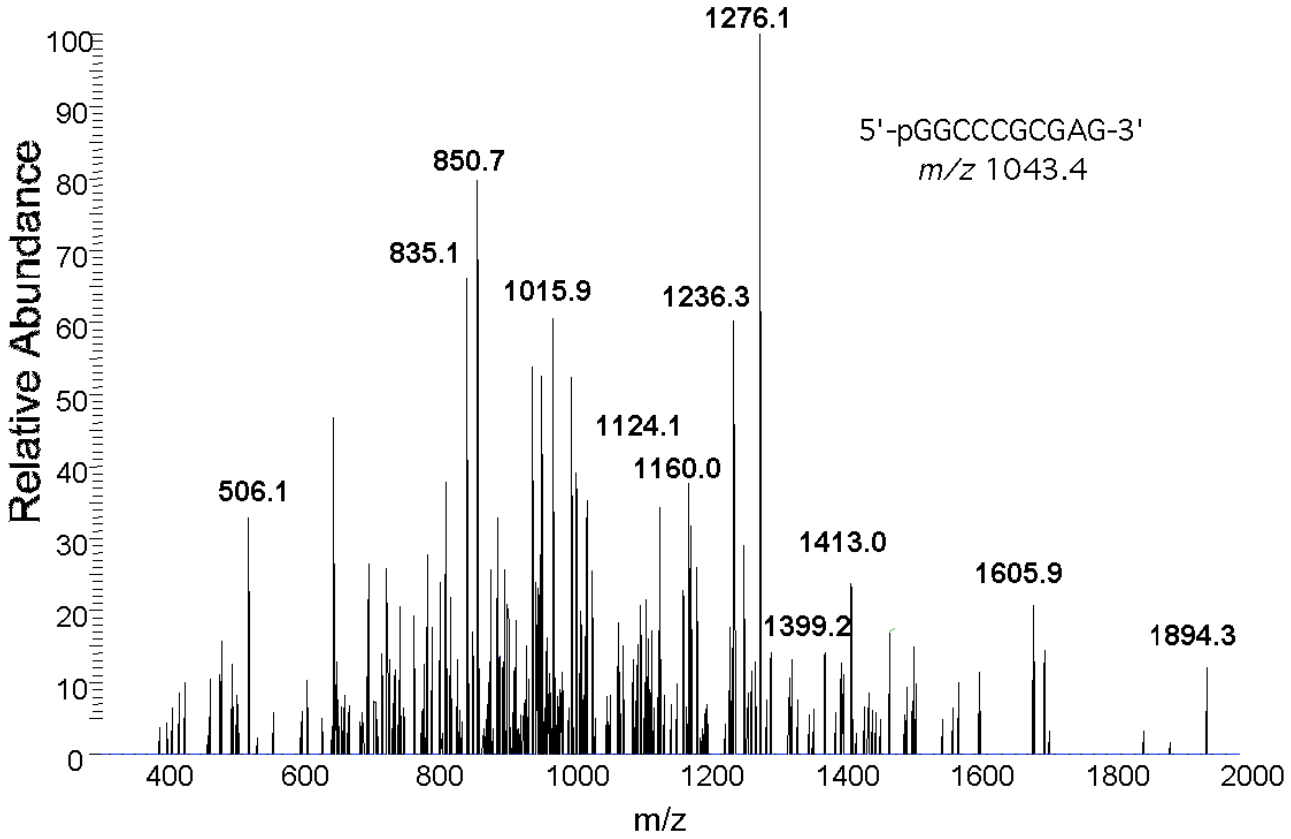

Figure S28. CID spectrum of the *m/z* 1043.4 product from the Dpo4 extension of oligonucleotide **1b**.

Table S5. Observed and calculated CID fragmentation of 5'-pGGCCCGCGAG-3'; *m/z* 1043.4 (M-3H)

Fragment assignment	observed	theoretical
5'-pG (a_2-B)	506.1	506.05
5'-pGG (a_3-B)	835.1	835.10
5'-pGGC (a_4-B)	1124.1	1124.14
5'-pGGCC (a_5-B)	1413.1	1413.19
5'-pGGCCC (a_6-B, -2)	850.7	850.61
5'-pGGCCCG (a_7-B, -2)	1015.9	1015.1
5'-pGGCCCGC (a_8-B, -2)	1160.0	1159.7
pGCCCGCGAG-3' (w_9, -2)	1399.2	1400.72
pCCCGCGAG-3' (w_8, -2)	1236.3	1236.20
pCGCGAG-3' (w_6)	1985.3	1895.31
pGCGAG-3' (w_4)	1605.9	1606.26
pCGAG-3' (w_4)	1276.1	1277.21

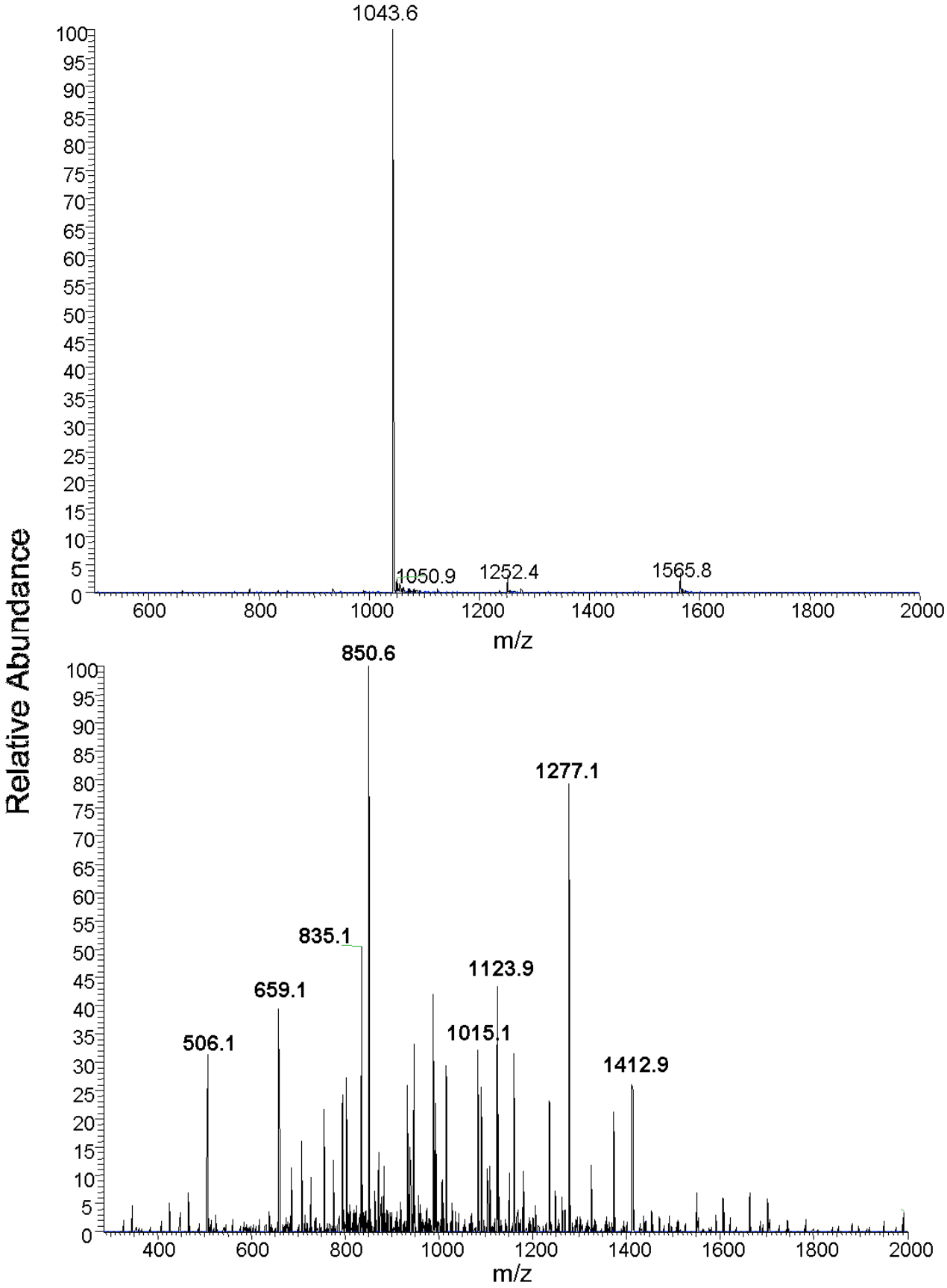

Figure S29. TIC (top) and CID (bottom) spectra of an authentic sample of 5'-pGGCCCGCGAG-3'; *m/z* 1043.4 (M-3H)

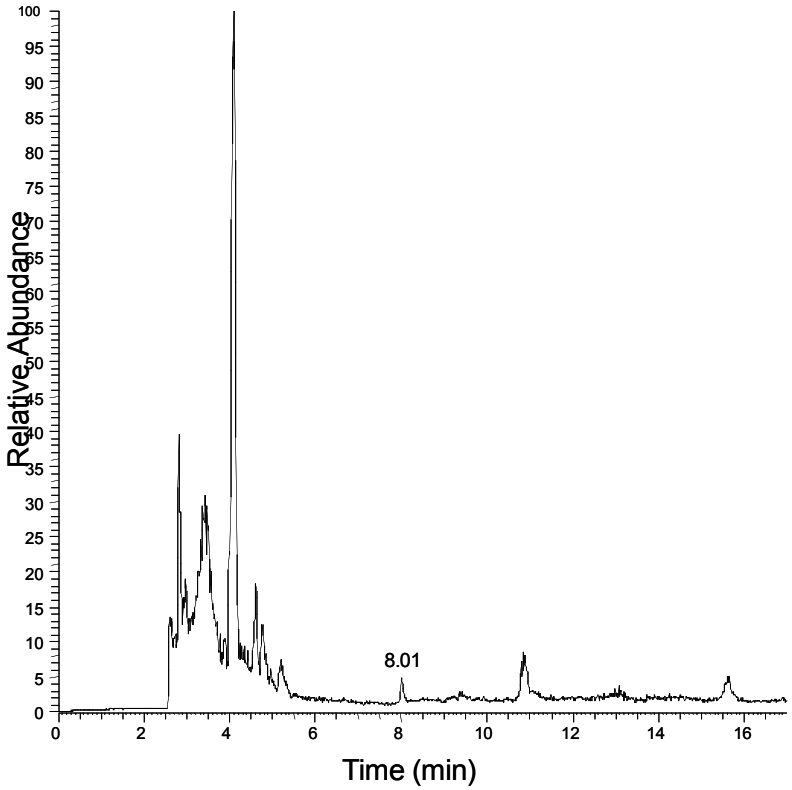

Figure S30. LC-ESI-MS/MS analysis of the Dpo4 extension of oligonucleotide **2b**

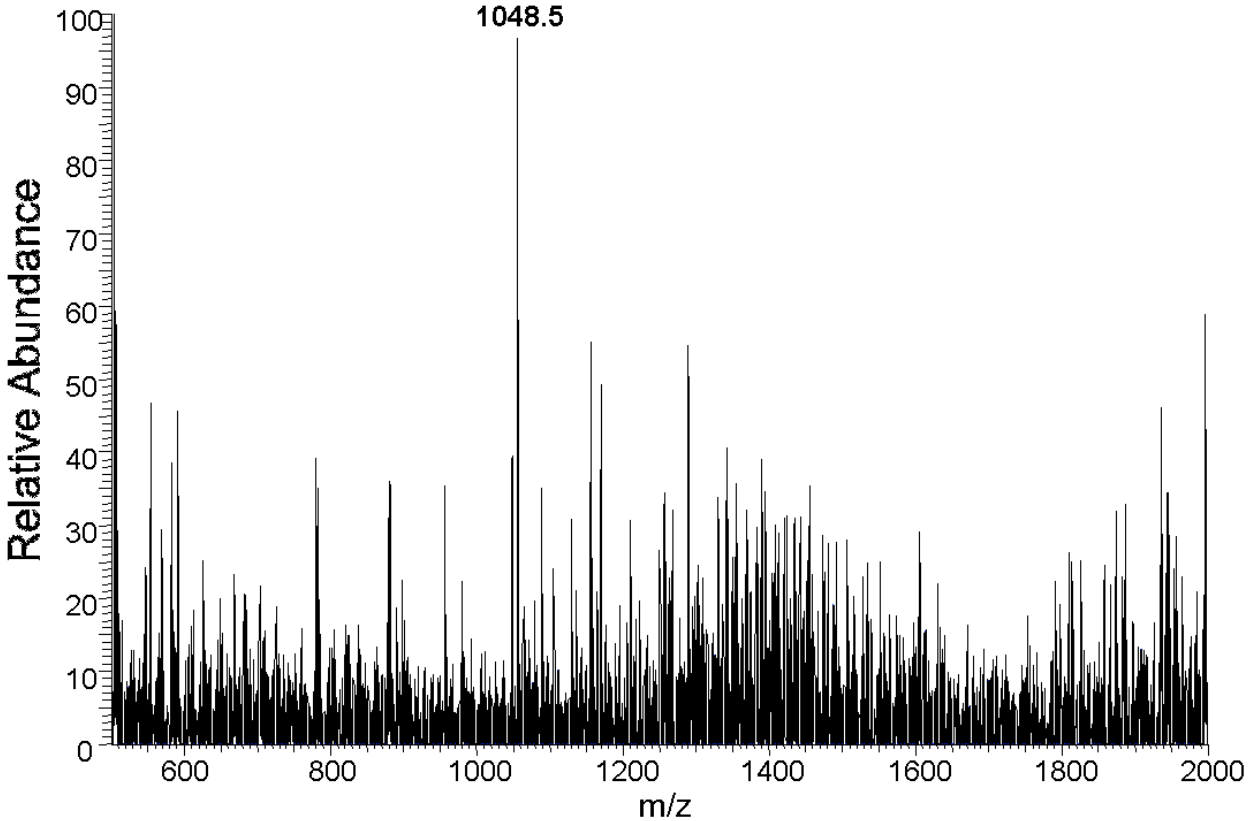

Figure S31. TIC spectrum of the Dpo4 extension products from oligonucleotide **2b**.

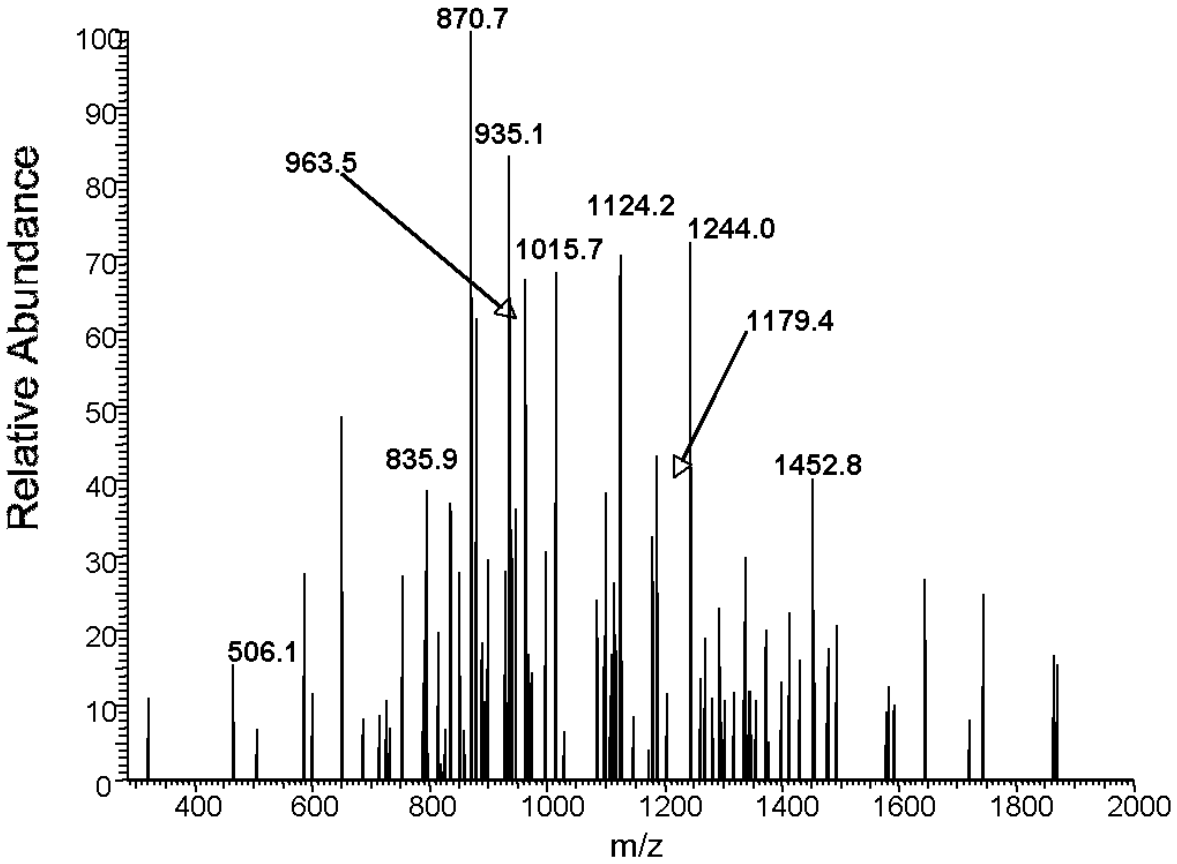

Figure S32. CID spectrum of the *m/z* 1048.5 products from the Dpo4 extension of oligonucleotide **2b**.

Table S6. Observed and calculated CID fragmentation of 5'-pGGCGCCGAGT-3' (*m/z* 1048.5)

Fragment assignment	observed	theoretical
5'-pG (a_2-B)	506.1	506.05
5-pGG (a_3-B)	835.9	835.10
5'-pGGC (a_4-B)	1124.2	1124.14
5'-pGGCG (a_5-B)	1452.8	1453.20
5'-pGGCGC (a_6-B, -2)	870.7	870.62
5'-pGGCGCC (a_7-B, -2)	1015.7	1015.14
5'-pGGCGCCG (a_8-B, -2)	1179.4	1179.67
pCGCCGAGT-3' (w_8, -2)	1244.0	1243.70
pCCGAGT-3' (w_6, -2)	935.1	934.65
pAGT-3' (w_3)	963.5	963.16
pGT-3' (w_2)	650.1	650.10

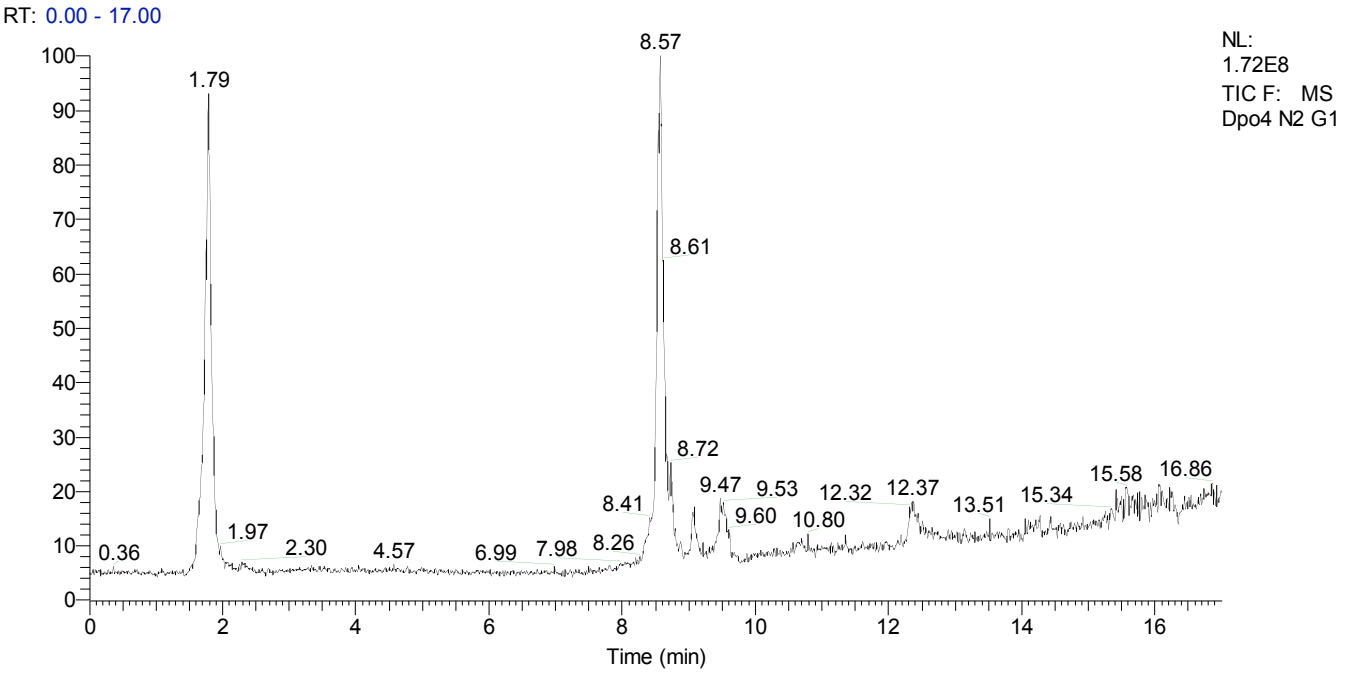

Figure S33. LC-ESI-MS/MS analysis of the Dpo4 extension of oligonucleotide **1c**.

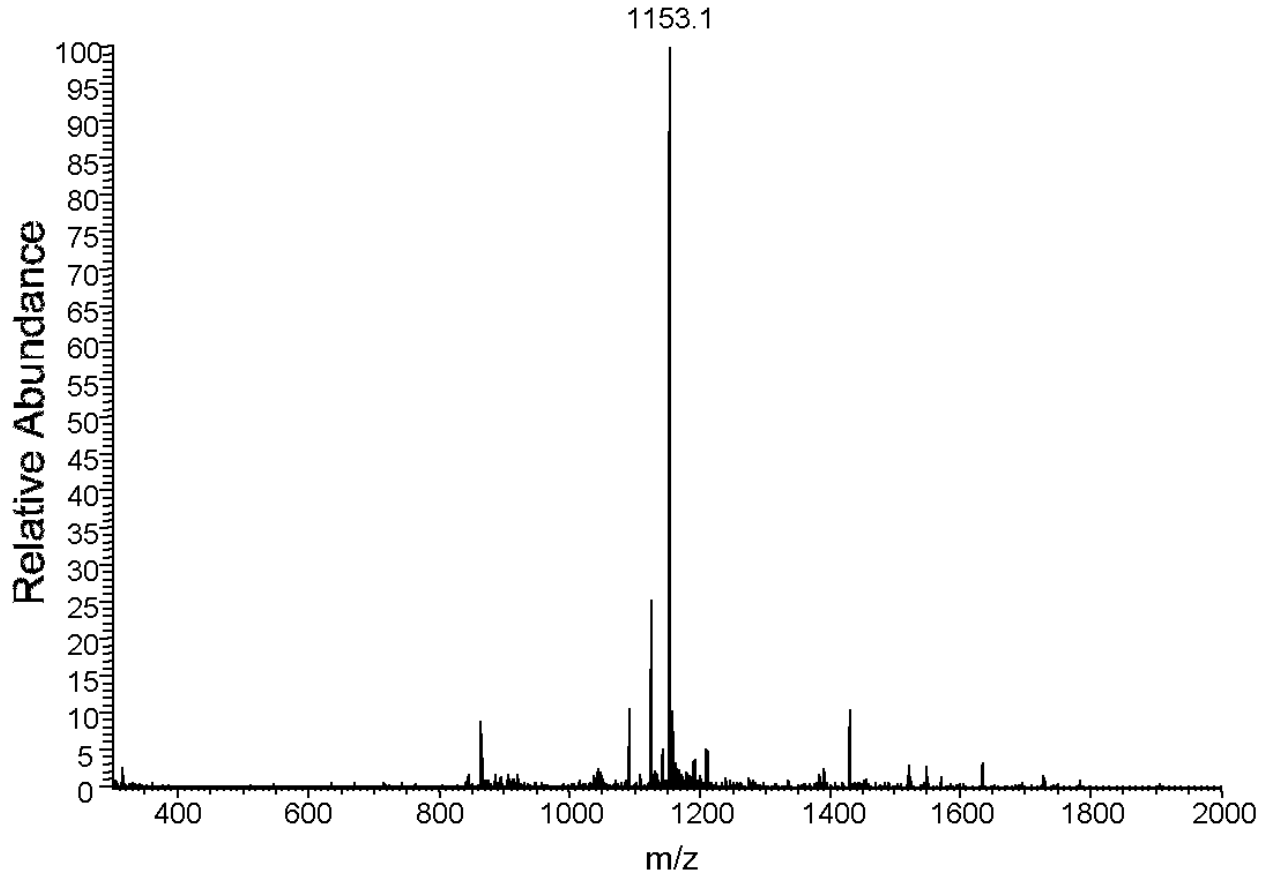

Figure S34. TIC spectrum of the Dpo4 extension products from oligonucleotide **1c**.

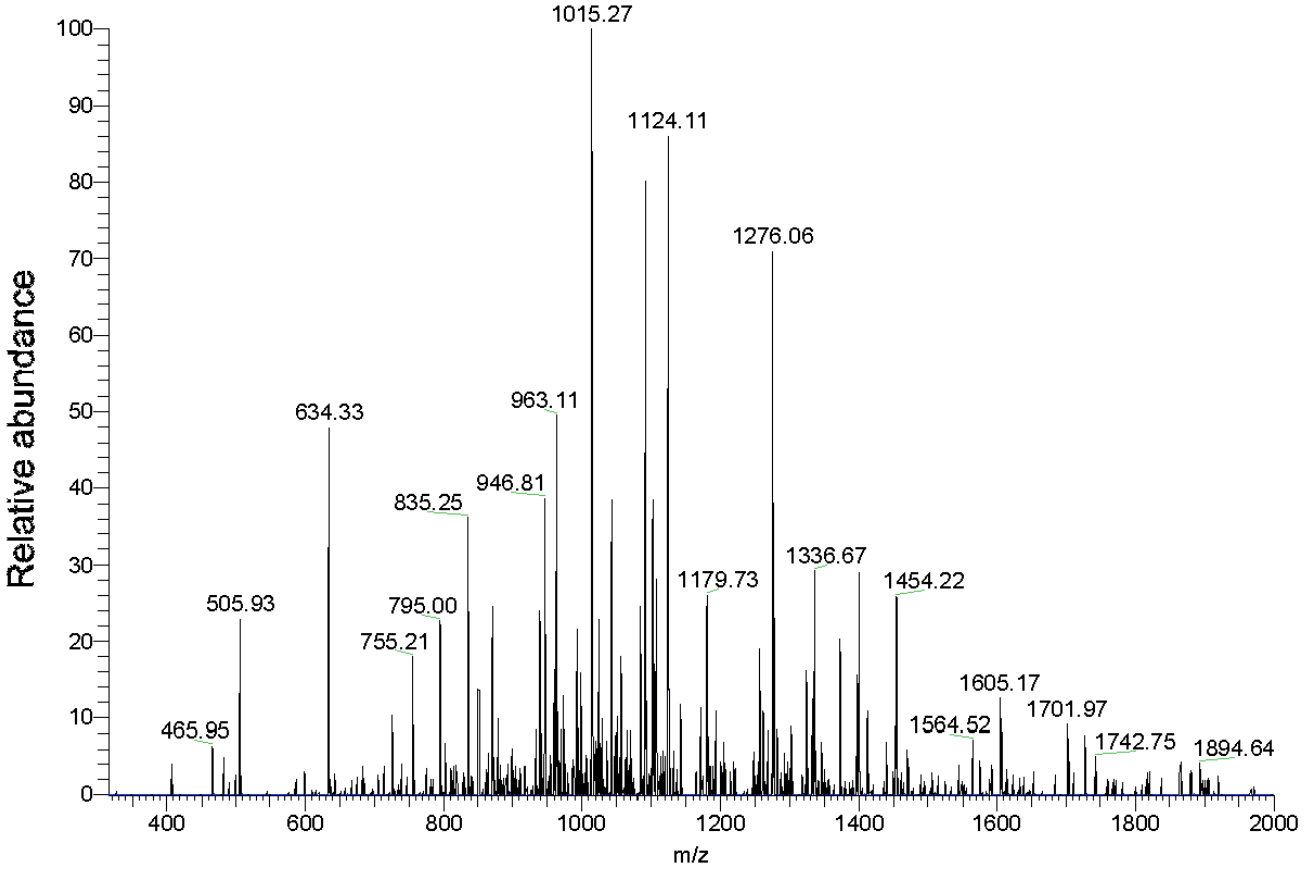

Figure S35. CID spectrum of the *m/z* 1153.1 products from the Dpo4 extension of oligonucleotide **1c**.

Table S7. Observed and calculated CID fragmentation of 5'-pGGCGCCGAGTA-3' (*m/z* 1153.1)

Fragment assignment	observed	theoretical
5'-pG (a_2-B)	506.93	506.05
5'-pGG (a_3-B)	835.3	835.10
5'-pGGC (a_4-B)	1124.1	1124.14
5'-pGGCG (a_5-B)	1454.2	1453.20
5'-pGGCGC (a_6-B)	1742.7	1742.24
(a_6-B, -2)	870.8	870.6
5'-pGGCGCC (a_7-B, -2)	1015.3	1015.14
5'-pGGCGCCG (a_8-B, -2)	1179.7	1179.67
5'-pGGCGCCGA (a_9-B, -2)	1336.7	1336.20
pGCGCCGAGTA-3' (w_8, -2)	1400.7	1400.22
pCGCCGAGTA-3' (w_8, -2)	1256.2	1255.70
pGCCGAGTA-3' (w_7, -2)	1091.4	1091.18
pCCGAGTA-3' (w_6, -2)	946.8	946.65
pGAGTA-3' (w_5)	1605.7	1605.27
pAGTA-3' (w_4)	1276.0	1276.21
pGTA-3' (w_3)	963.1	963.16
pTA-3' (w_2)	634.3	634.10

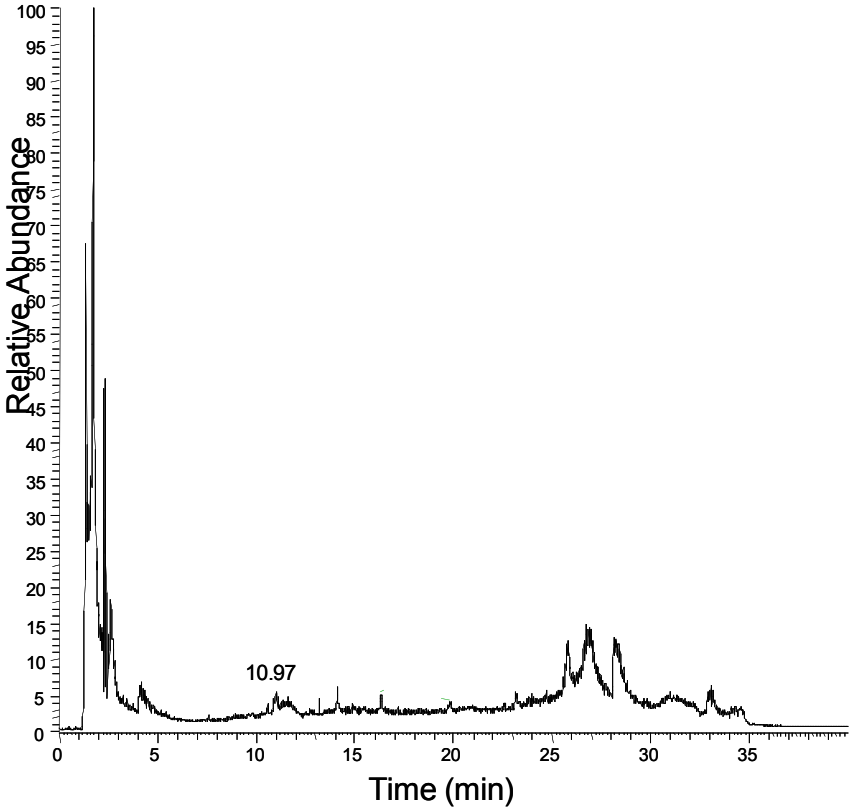

Figure S36. LC-ESI-MS/MS analysis of the Dpo4 extension of oligonucleotide **2c**.

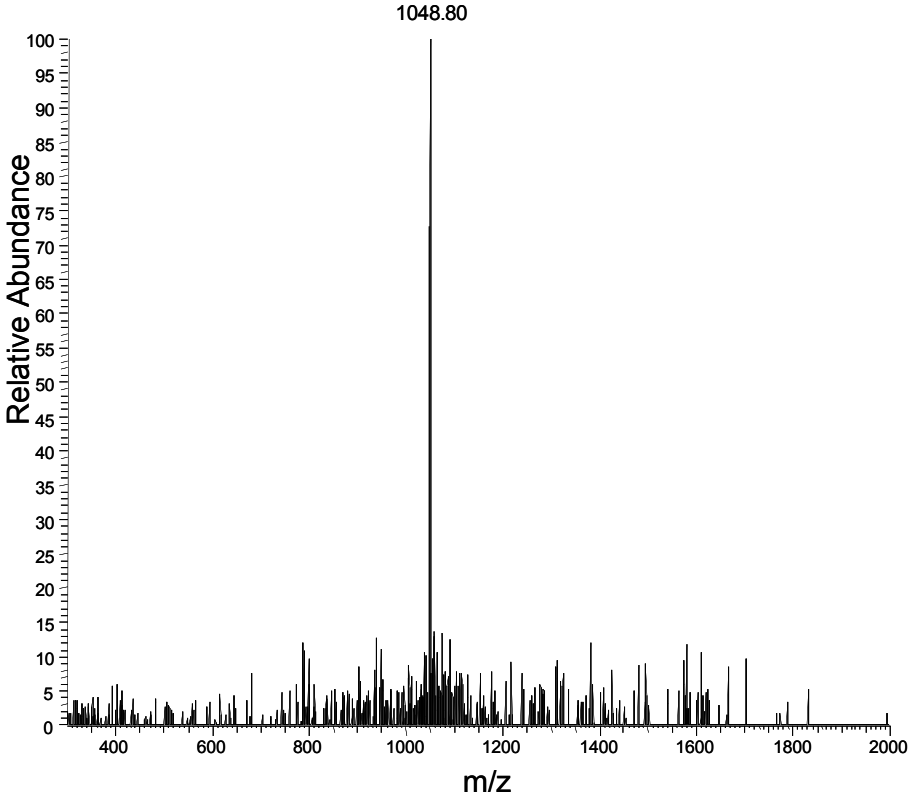

Figure S37. TIC spectrum of the Dpo4 extension products from oligonucleotide **2c**.

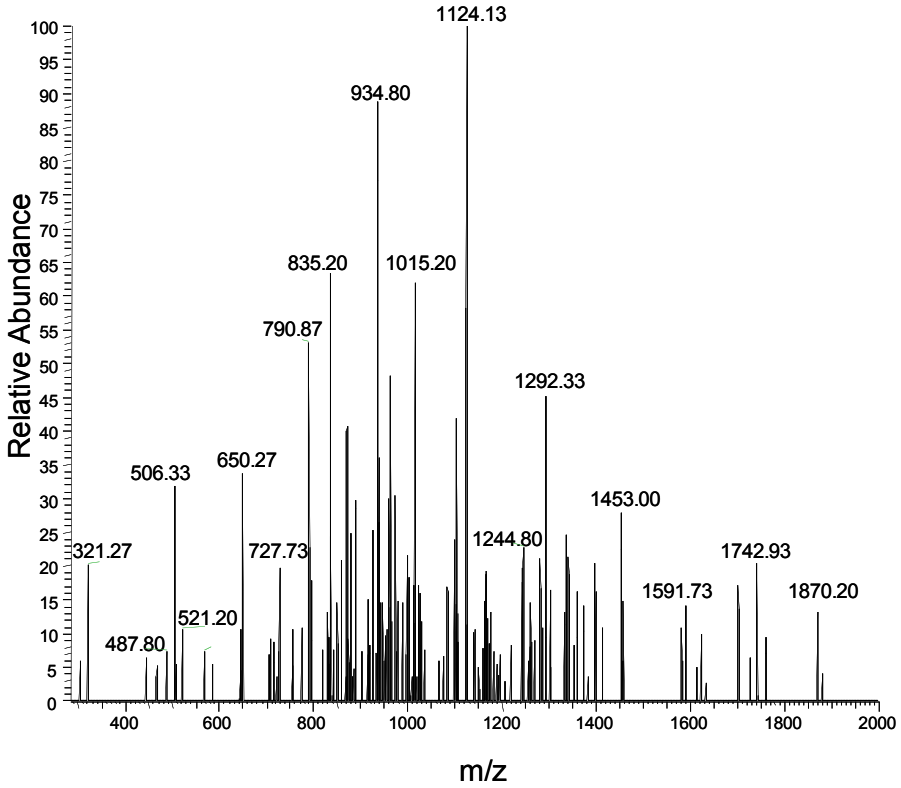

Figure S38. CID spectrum of the *m/z* xxxx products from the Dpo4 extension of oligonucleotide **2b**.

Table S8. Observed and calculated CID fragmentation of 5'-pGGCGCCGAGT-3' (*m/z* 1048.8)

Fragment assignment	observed	theoretical
5'-pG (a_2-B)	506.3	506.05
5'-pGG (a_3-B)	835.2	835.10
5'-pGGC (a_4-B)	1124.1	1124.14
5'-pGGCG (a_5-B)	1453.0	1453.20
5'-pGGCGC (a_6-B)	1742.9	1742.24
(a_6-B, -2)	870.5	870.62
5'-pGGCGCC (a_7-B, -2)	1015.2	1015.14
pCGCCGAGT-3' (w_8, -2)	1244.8	1243.7
pGCCGAGT-3' (w_7, -2)	1099.1	1099.17
pCCGAGT-3' (w_6)	1870.2	1870.30
(w_6, -2)	934.8	934.65
pCGAGT-3' (w_5, -2)	790.9	790.12
pGAGT-3' (w_4)	1292.3	1292.21
pAGT-3' (w_3)	963.4	963.16
pGT-3' (w_2)	650.2	650.10
pT-3' (w_1)	321.3	321.05