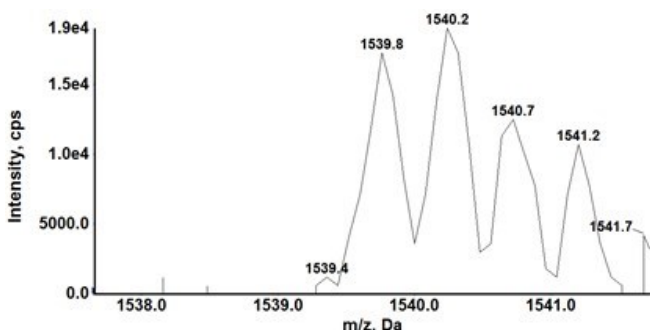


## CHEMICAL SELECTIVITY OF NUCLEOBASE ADDUCTION RELATIVE TO IN VIVO MUTATION SITES ON EXON 7 FRAGMENT OF P53 TUMOR SUPPRESSOR GENE

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### SUPPORTING INFORMATION



**Figure S1.** Isotopic distribution pattern for ss-DNA Fragment 1,  $m/z$  1540.5  $z=-2$ , measured on a Qtrap mass spectrometer

**Table S1:** Calculated multiple charged species for standard and single adducted ss-Fragment 1.

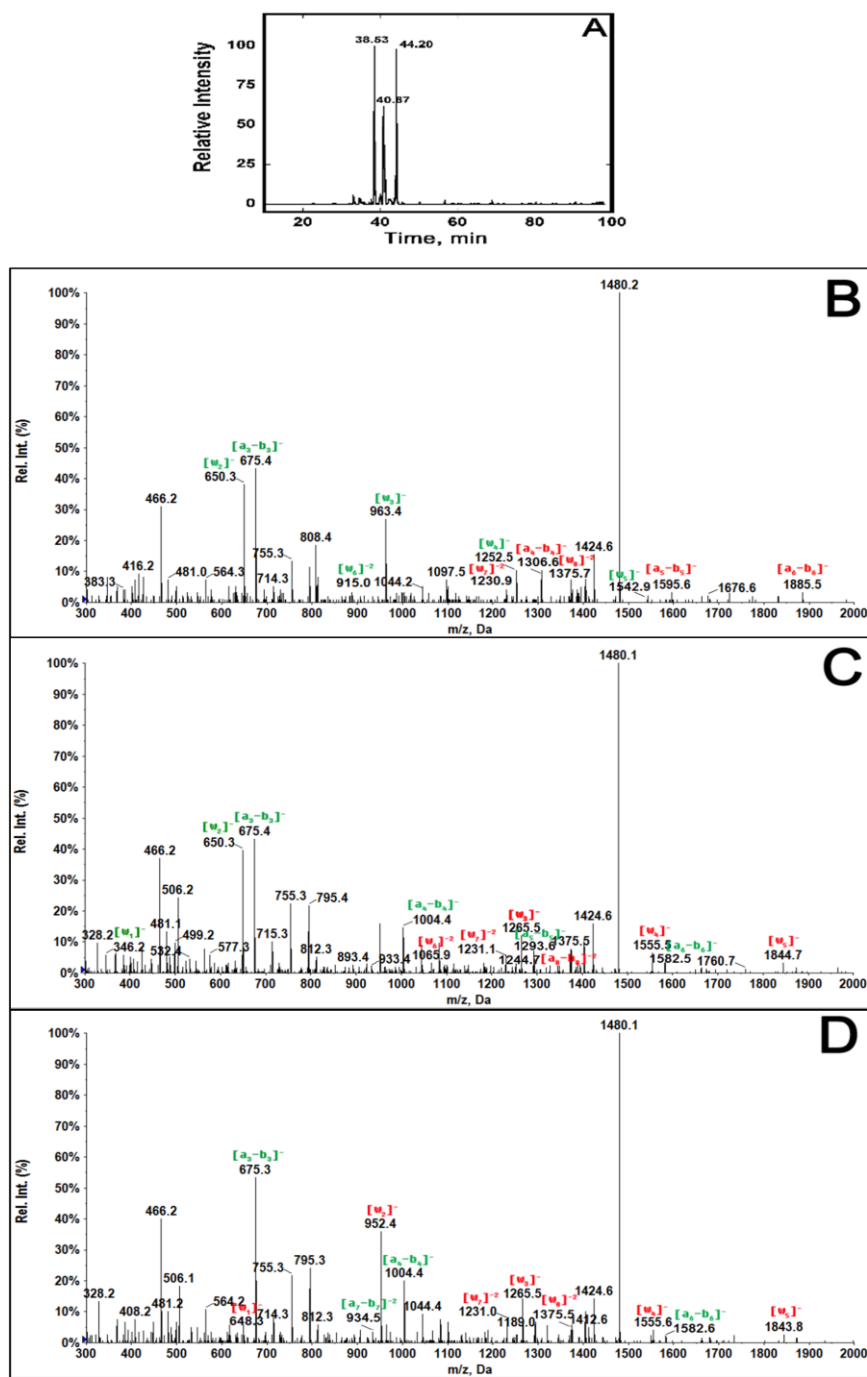
ss-Fragment 1 : GGCGGCATG		
Charge	m/z	
	Standard	Singly Adducted
-1	2778.854	3081.177
-2	1388.923	1540.084
-3	925.612	1026.386
-4	693.957	769.538
-5	554.964	615.429
-6	462.302	512.689
-7	396.115	439.304
-8	346.474	384.264

Singly adducted ss-DNA Fragment 4 has  $m/z$  of 1480.2 with a charge of -2. Extracted ion chromatogram (XIC) of 1480.2 is as shown in Figure S2A. XIC of 1480.2 showed three major peaks indicating that there are three major adducts on ss-DNA Fragment 4, the complement of fragment 1. MSMS spectra for singly adducted ss-DNA Fragment 4,  $m/z$  1480.2 is as shown in Figure S2B for Peak 1. All  $a_n$ - $b_n$  ions up to  $a_3$ - $b_3$  have  $m/z$  similar to that of standard. Increase in  $m/z$  was observed for  $a_4$ - $b_4$ ,  $a_5$ - $b_5$  and  $a_6$ - $b_6$ . This indicates that the possible modification is on base 3, (CCG\*CCCATG). This was further confirmed with  $w_n$  ions. Increase in  $m/z$  for  $w_7$  and  $w_8$  ions and all ions below  $w_6$  have  $m/z$  similar to that of standard. Table S2 shows the  $m/z$  for standard and adducted ss-DNA Fragment 4.

MSMS spectra for singly adducted ss-DNA Fragment 4,  $m/z$  1480.2 is as shown in Figure S2C for Peak 2. All  $a_n$ - $b_n$  ions up to  $a_7$ - $b_7$  have  $m/z$  similar to that of standard. Increase in  $m/z$  was observed for  $a_8$ - $b_8$ . This indicates that the possible modification is on base 7, (CCGCCCA\*TG). This was further confirmed with  $w_n$  ions. Increase in  $m/z$  for  $w_3$ ,  $w_4$ ,  $w_5$ ,  $w_6$ ,  $w_7$  and  $w_8$  ions and ions  $w_1$  and  $w_2$

have  $m/z$  similar to that of standard. Table S2 shows the  $m/z$  for standard and adducted ss-DNA Fragment 4.

MSMS spectra for singly adducted ss-DNA Fragment 4,  $m/z$  1480.2 is as shown in Figure S2D for Peak 3. All  $a_n$ - $b_n$  ions have  $m/z$  similar to that of standard. This indicates that the possible modification is on base 9, (CCGCCCATG\*). This was further confirmed with  $w_n$  ions showing increase in  $m/z$  for all  $w_n$  ions. Table S2 shows the  $m/z$  for standard and adducted fragment 4.

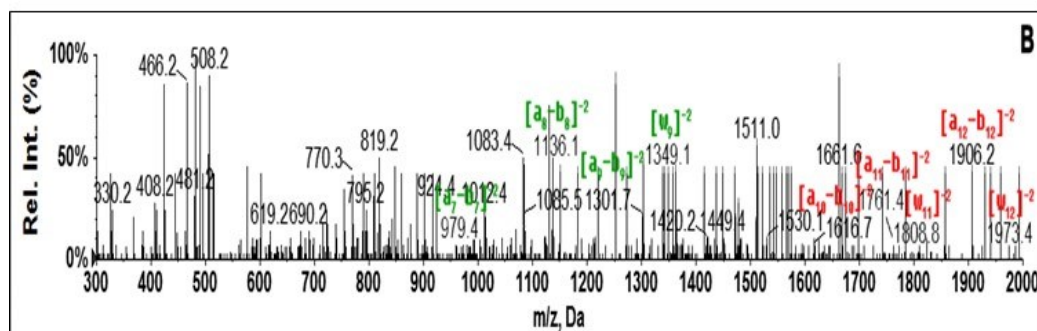
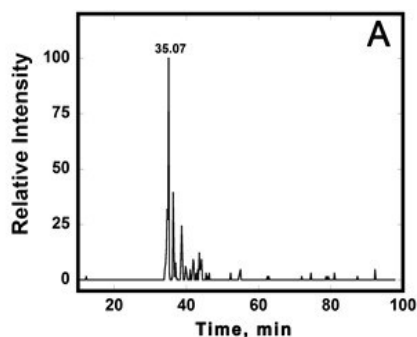


**Figure S2.** LC-MS/MS of ss Fragment 4 (A) Extracted ion chromatogram of singly adducted ss Fragment 4 fragment with  $m/z$  1480.2. (B) MSMS spectra of Peak 1 (C) MSMS spectra of Peak 2 (D) MSMS spectra of Peak 3 showing the obtained  $a_n$ - $b_n$  and  $w_n$  ions. Ions with  $m/z$  similar to standard are shown in green and ions with increased  $m/z$  shown in red.

**Table S2:** Calculated m/z for standard and singly adducted DNA fragments of ss-DNA Fragment 4. (m/z highlighted in red were the ions with increased m/z compared to that of standard corresponding to BPDE adducted)

Fragment	m/z			
	Standard	Peak1	Peak 2	Peak 3
a <sub>2</sub> -b <sub>2</sub>	[386.2] <sup>-</sup>	[426.2] <sup>-</sup>	[386.2] <sup>-</sup>	[386.2] <sup>-</sup>
a <sub>3</sub> -b <sub>3</sub>	[675.4] <sup>-</sup>	[675.4] <sup>-</sup>	[675.4] <sup>-</sup>	[675.4] <sup>-</sup>
a <sub>4</sub> -b <sub>4</sub>	[1004.4] <sup>-</sup>	[1306.6] <sup>-</sup>	[1004.4] <sup>-</sup>	[1004.4] <sup>-</sup>
a <sub>5</sub> -b <sub>5</sub>	[1293.8] <sup>-</sup>	[1595.6] <sup>-</sup>	[1293.8] <sup>-</sup>	[1293.8] <sup>-</sup>
a <sub>6</sub> -b <sub>6</sub>	[1583.0] <sup>-</sup>	[1885.5] <sup>-</sup>	[1582.5] <sup>-</sup>	[1582.6] <sup>-</sup>
a <sub>7</sub> -b <sub>7</sub>	[1872.2] <sup>-2</sup>	n/d	n/d	[934.5] <sup>-2</sup>
a <sub>8</sub> -b <sub>8</sub>	[1092.2] <sup>-2</sup>	n/d	[1244.7] <sup>-2</sup>	n/d
w <sub>1</sub>	[346.2] <sup>-2</sup>	[346.2] <sup>-2</sup>	[346.2] <sup>-2</sup>	[648.23] <sup>-</sup>
w <sub>2</sub>	[650.4] <sup>-</sup>	[650.3] <sup>-</sup>	[650.3] <sup>-</sup>	[952.4] <sup>-</sup>
w <sub>3</sub>	[963.6] <sup>-</sup>	[963.4] <sup>-</sup>	[1265.5] <sup>-</sup>	[1265.6] <sup>-2</sup>
w <sub>4</sub>	[1252.8] <sup>-</sup>	[1252.5] <sup>-</sup>	[1555.5] <sup>-</sup>	[1554.6] <sup>-</sup>
w <sub>5</sub>	[1541.9] <sup>-</sup>	[1542.9] <sup>-</sup>	[1844.7] <sup>-</sup>	[1843.8] <sup>-</sup>
w <sub>6</sub>	[1831.2] <sup>-</sup>	[915.0] <sup>-2</sup>	[1066.6] <sup>-2</sup>	[1066.6] <sup>-2</sup>
w <sub>7</sub>	[1079.7] <sup>-2</sup>	[1230.9] <sup>-2</sup>	[1231.1] <sup>-2</sup>	[1231.0] <sup>-2</sup>
w <sub>8</sub>	[1224.3] <sup>-2</sup>	[1375.7] <sup>-2</sup>	[1375.6] <sup>-2</sup>	[1375.5] <sup>-2</sup>

Singly adducted fragment of ss-DNA Fragment 2 has an m/z of 1511.0 with a charge of -4. Extracted ion chromatogram of 1511.0 is as shown in Figure S3A. XIC of 1511.0 show one major peak indicating that there is one major adduct on ss-DNA Fragment 2.



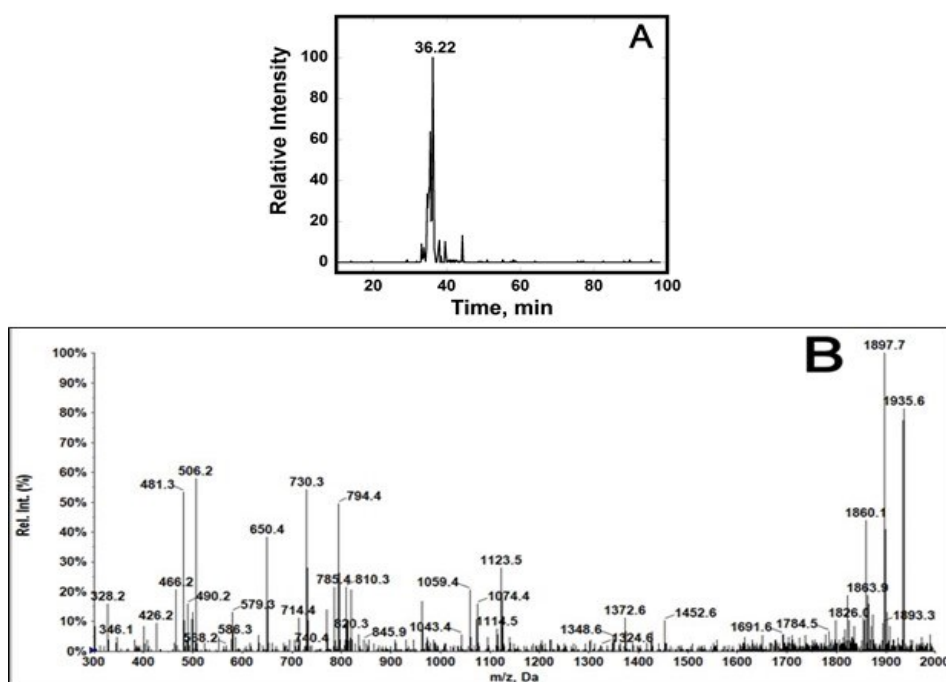
**Figure S3.** LC-MS/MS of ss-DNA fragment 2 (A) Extracted ion chromatogram of singly adducted ss-DNA Fragment 2 fragment, m/z 1511.0.

(B) MSMS spectra of fragment ion 1511.0 showing the obtained a<sub>n</sub>-b<sub>n</sub> and w<sub>n</sub> ions. Ions with m/z similar to standard are shown in green and ions with increased m/z shown in red.

MSMS spectra for singly adducted ss-DNA Fragment 2, m/z 1511.0 is as shown in Figure S3B. All  $a_n$ - $b_n$  ions up to  $a_9$ - $b_9$  have m/z similar to that of standard. Increase in m/z was observed for  $a_{10}$ - $b_{10}$ . This indicates that the possible modification is on base 9, (AACCGGAGG\*CCCATCCTCA). This was further confirmed with  $w_n$  ions. Increase in m/z for  $w_{11}$ ,  $w_{12}$ , and  $w_{13}$  ions and ions below  $w_{10}$  have m/z similar to that of standard. Table S3 shows the m/z for standard and adducted ss-DNA Fragment 2.

**Table S3:** Calculated m/z for standard and singly adducted DNA fragments of ss-DNA Fragment 2. (m/z highlighted in red were the ions with increased m/z compared to that of standard corresponding to BPDE adducted)

Fragment Ion	m/z	
	Standard	Singly adducted
$a_7$ - $b_7$	[979.4] <sup>-2</sup>	[979.4] <sup>-2</sup>
$a_8$ - $b_8$	[1136.1] <sup>-2</sup>	[1136.1] <sup>-2</sup>
$a_9$ - $b_9$	[1301.0] <sup>-2</sup>	[1301.0] <sup>-2</sup>
$a_{10}$ - $b_{10}$	[1465.5] <sup>-2</sup>	[1616.7] <sup>-2</sup>
$a_{11}$ - $b_{11}$	[1073.0] <sup>-3</sup>	[1761.4] <sup>-2</sup>
$a_{12}$ - $b_{12}$	[1169.4] <sup>-3</sup>	[1906.2] <sup>-2</sup>
$w_8$	[1204.4] <sup>-2</sup>	[1204.4] <sup>-2</sup>
$w_9$	[1349.1] <sup>-2</sup>	[1349.1] <sup>-2</sup>
$w_{10}$	[1492.9] <sup>-2</sup>	[1493.2] <sup>-2</sup>
$w_{11}$	[1657.5] <sup>-2</sup>	[1808.8] <sup>-2</sup>
$w_{12}$	[1214.4] <sup>-3</sup>	[1973.4] <sup>-2</sup>

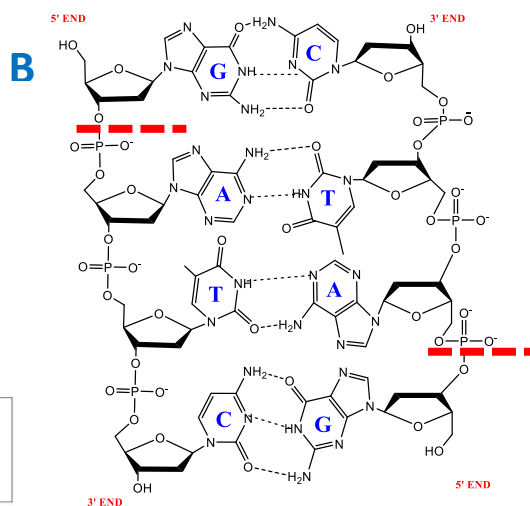
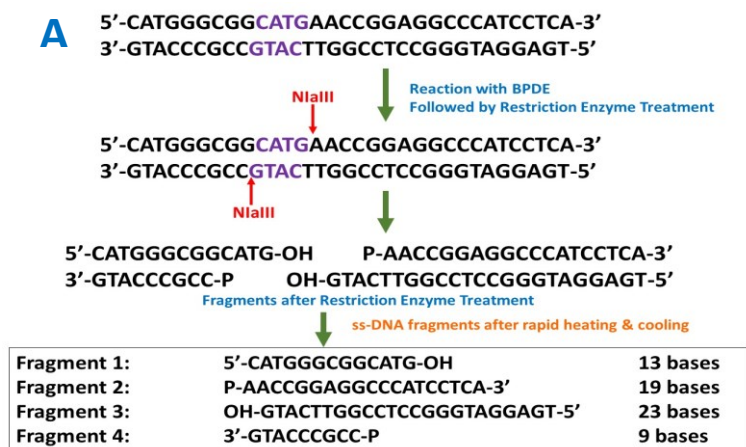


**Figure S4.** LC-MS/MS of ss-DNA Fragment 3 (A) Extracted ion chromatogram of singly adducted ss-DNA Fragment 3, m/z 1935.5. (B) MSMS spectra of fragment ion of m/z, 1935.5 charge -4 showing the obtained  $a_n$ - $b_n$  and  $w_n$  ions. Ions with m/z similar to standard are shown in green and ions with increased m/z shown in red.

Singly adducted ss-DNA Fragment 3 has m/z of 1935.5 with a charge of -4. Extracted ion chromatogram of 1935.5 is as shown in figure S4A. XIC of 1935.5 show one major peak indicating that there is one major adduct on ss-DNA Fragment 4.

MSMS spectra for singly adducted ss-DNA Fragment 3, m/z 1935.5 is as shown in Figure S4B. Increase in m/z for  $w_n$  ions  $w_{20}$ ,  $w_{21}$ ,  $w_{22}$  and  $w_{23}$  indicate that the modification is on 5<sup>th</sup> base (GTGAG\*GATGGGCTCCGGTTCATG).

### 32 base pair DNA DATA



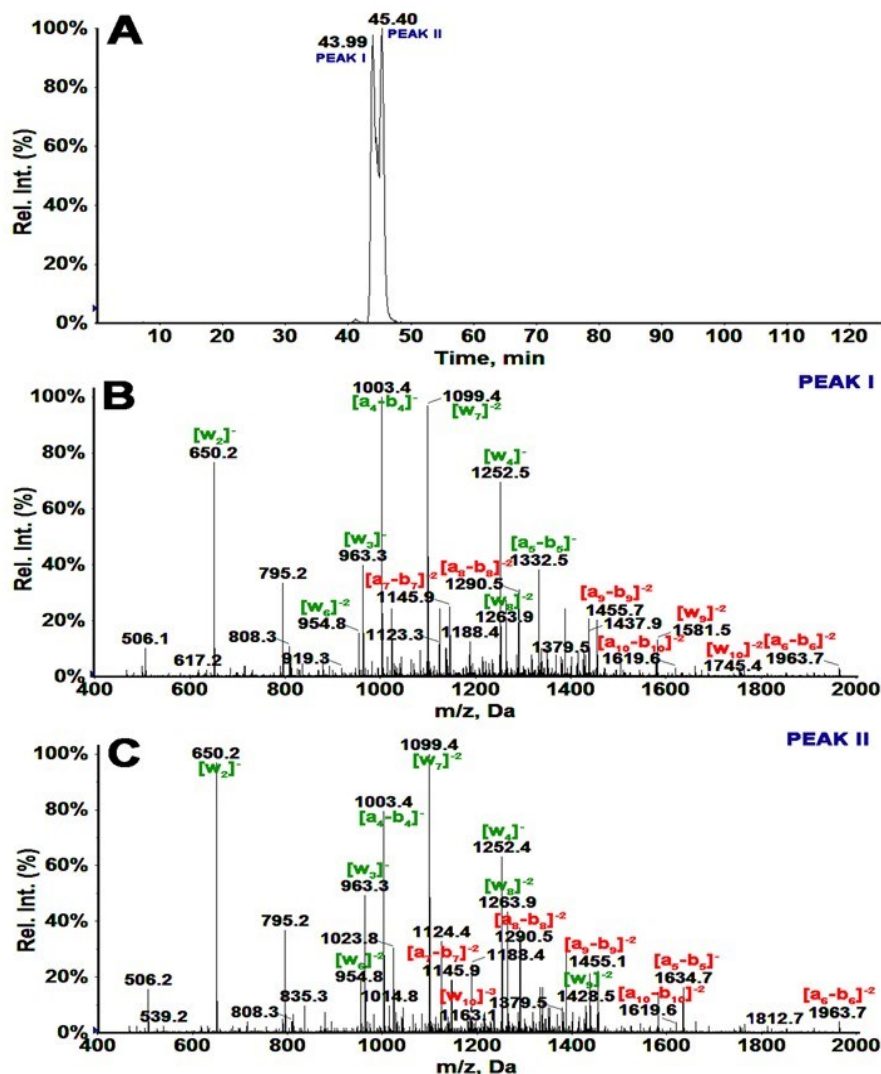
**Scheme S1.** A) Protocol for reaction of 32 base pairs DNA fragment with BPDE followed by restriction enzyme treatment and possible fragments. B) Example of bond breaking between O and P if restriction enzyme acts between G and A.

**Table S4:** Calculated m/z for standard and singly adducted DNA fragments obtained after restriction enzyme treatment of 32 base pair DNA (A) Fragment 1 (B) Fragment 2 (C) Fragment 3 (D) Fragment 4. m/z highlighted in red were the ions detected in MS spectrum.

(A) Fragment 1 5'-CATGGGCGGCATG-OH			(B) Fragment 2 P-AACCGGAGGCCATCCTCA-OH		
Charge	Standard	Single adducted	Charge	Standard	Single adducted
-1	4014.656	4316.979	-1	5821.771	6124.094
-2	2006.824	2157.986	-2	2910.381	3061.543
-3	1337.546	1438.320	-3	1939.918	2040.692
-4	1002.908	1078.489	-4	1454.686	1530.267
-5	802.124	862.589	-5	1163.547	1224.012
Charges up to -12 are possible only few shown here			Charges up to -18 are possible only few shown here		

(C) Fragment 3 OH-GTACTTGGCCTCCGGGTAGGAGT-OH			(D) Fragment 4 OH-GTACCCGCC-P		
Charge	Standard	Single adducted	Charge	Standard	Single adducted
-1	7110.654	7412.977	-1	2738.759	3041.082
-2	3554.823	3705.985	-2	1368.875	1520.037
-3	2369.546	2470.320	-3	912.247	1013.021
-4	1776.907	1852.488	-4	683.933	759.514
-5	1421.324	1481.789	Charges up to -8 are possible only few shown here		
-6	1184.269	1234.656			



**Figure S5.** LC-MS of ds-32 bp exon 7 probe: (A) Extracted ion chromatogram of singly adducted fragment 1, m/z 1438.2. (B) MSMS spectra of Peak 1 (C) MSMS spectra of Peak 2 showing the obtained  $a_n$ - $b_n$  and  $w_n$  ions. Ions with m/z similar to standard are shown in green and ions with increased m/z shown in red.

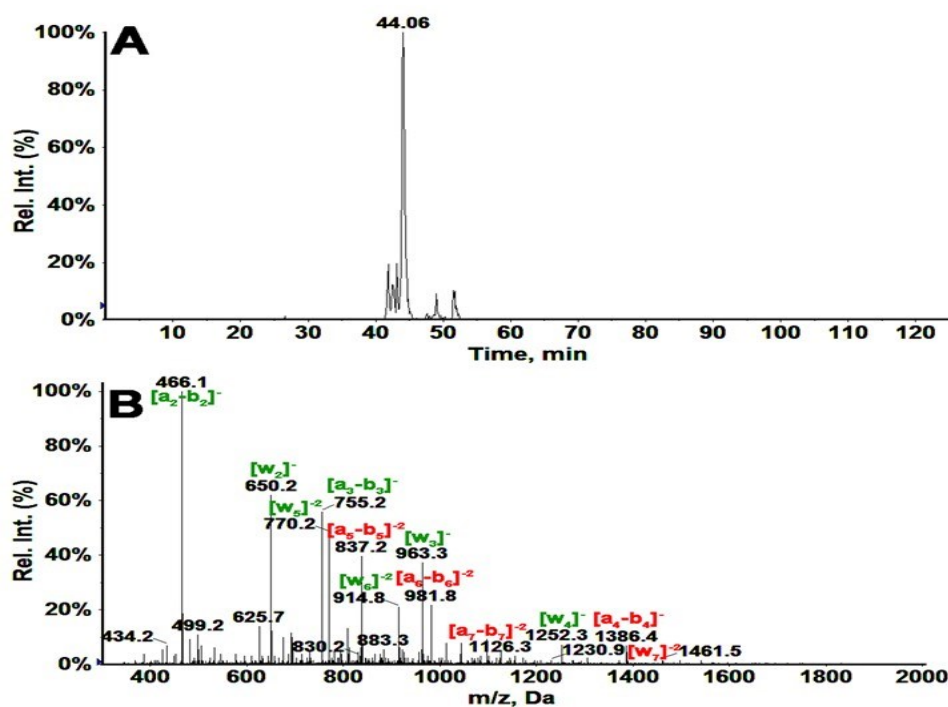
Singly adducted fragment 1 has an m/z of 1438.2 with a charge of -3. Extracted ion chromatogram of 1438.2 is shown in Figure S6A. XIC of 1223.8 show two major peaks indicating that there are two major adduct on Fragment 1.

MSMS spectra for singly adducted Fragment 1, m/z 1438.2 is as shown in Figure S6B for Peak 1. All  $a_n$ - $b_n$  ions up to  $a_5$ - $b_5$  have m/z similar to that of standard. Increase in m/z was observed for  $a_6$ - $b_6$ ,  $a_7$ - $b_7$ ,  $a_8$ - $b_8$ . This indicates that the possible modification is on base 5, (CATGG\*GCGGCATG). This was further confirmed with  $w_n$  ions. Increase in m/z for  $w_9$  and  $w_{10}$  ions and all ions below  $w_8$  have m/z similar to that of standard. Table showing the m/z for standard and adducted Fragment 1 is as shown in Table S5.

MSMS spectra for singly adducted Fragment 1, m/z 1438.2 is as shown in Figure S6C for Peak 2. All  $a_n$ - $b_n$  ions up to  $a_5$ - $b_5$  have m/z similar to that of standard. Increase in m/z was observed for  $a_5$ - $b_5$ ,  $a_6$ - $b_6$ ,  $a_7$ - $b_7$  and  $a_8$ - $b_8$ . This indicates that the possible modification is on base 4, (CATG\*GGCGGCATG). This was further confirmed with  $w_n$  ions. Increase in m/z for  $w_{10}$  ion and all ions below  $w_9$  have m/z similar to that of standard. Table showing the m/z for standard and adducted Fragment 1 is as shown in Table S5.

**Table S5.** Calculated m/z for standard and singly adducted DNA Fragment 1. (m/z highlighted in red were the ions with increased m/z compared to that of standard corresponding to BPDE adducted)

Fragment ion	m/z		
	Unadducted	Peak 1	Peak 2
$a_4-b_4^-$	[1003.4] <sup>-</sup>	[1003.4] <sup>-</sup>	[1003.4] <sup>-</sup>
$a_5-b_5^-$	[1332.5] <sup>-</sup>	[1332.5] <sup>-</sup>	[1634.7] <sup>-</sup>
$a_6-b_6^-$	[1661.6] <sup>-</sup>	[1963.7] <sup>-</sup>	[1963.7] <sup>-</sup>
$a_7-b_7^-$	[995.2] <sup>-2</sup>	[1145.9] <sup>-2</sup>	[1145.9] <sup>-2</sup>
$a_8-b_8^-$	[1139.5] <sup>-2</sup>	[1290.5] <sup>-2</sup>	[1290.5] <sup>-2</sup>
$a_9-b_9^-$	[1304.1] <sup>-2</sup>	[1455.7] <sup>-2</sup>	[1455.1] <sup>-2</sup>
$a_{10}-b_{10}^-$	[1468.5] <sup>-2</sup>	[1619.6] <sup>-2</sup>	[1619.6] <sup>-2</sup>
w <sub>2</sub>	[650.2] <sup>-</sup>	[650.2] <sup>-</sup>	[650.2] <sup>-</sup>
w <sub>3</sub>	[963.3] <sup>-</sup>	[963.3] <sup>-</sup>	[963.3] <sup>-</sup>
w <sub>4</sub>	[1252.5] <sup>-</sup>	[1252.5] <sup>-</sup>	[1252.5] <sup>-</sup>
w <sub>5</sub>	n/d	n/d	n/d
w <sub>6</sub>	[954.8] <sup>-2</sup>	[954.8] <sup>-2</sup>	[954.8] <sup>-2</sup>
w <sub>7</sub>	[1099.4] <sup>-2</sup>	[1099.4] <sup>-2</sup>	[1099.4] <sup>-2</sup>
w <sub>8</sub>	[1263.9] <sup>-2</sup>	[1263.9] <sup>-2</sup>	[1263.9] <sup>-2</sup>
w <sub>9</sub>	[1428.7] <sup>-2</sup>	[1581.5] <sup>-2</sup>	[1428.5] <sup>-2</sup>
w <sub>10</sub>	[1593.3] <sup>-2</sup>	[1745.4] <sup>-2</sup>	[1163.1] <sup>-3</sup>



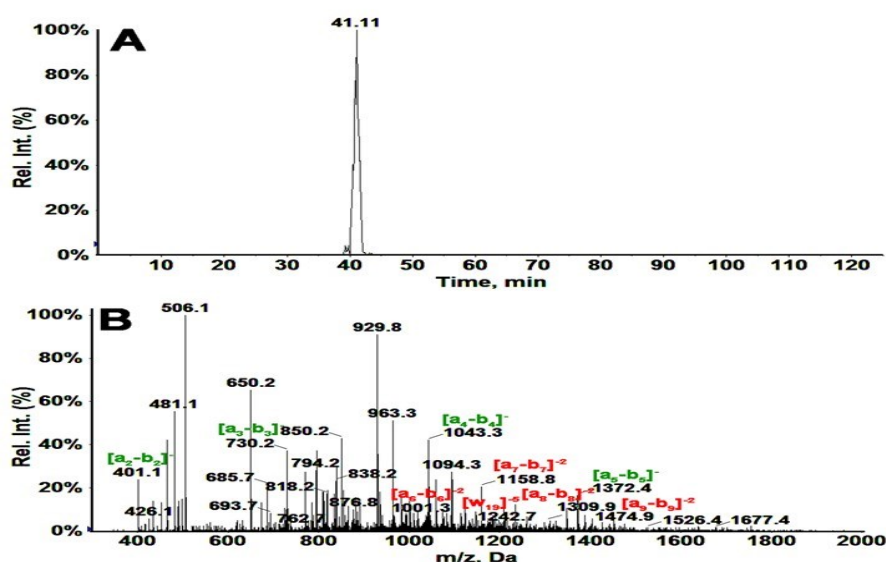
**Figure S6.** LC-MS of ds-32 bp exon 7 probe: (A) Extracted ion chromatogram of singly adducted Fragment 4, m/z 1012.6. (B) MSMS spectra of m/z 1012.6 showing the obtained a<sub>n</sub>-b<sub>n</sub> and w<sub>n</sub> ions. Ions with m/z similar to standard are shown in green and ions with increased m/z shown in red

Singly adducted Fragment 4 has an m/z of 1012.6 with a charge of -3. Extracted ion chromatogram of 1012.6 is as shown in Figure S7A. XIC of 1012.6 show one major peak indicating that there is one major adduct on Fragment 4.

MSMS spectra for singly adducted Fragment 4, m/z 1012.6 is as shown in Figure S7B. All  $a_n$ - $b_n$  ions up to  $a_3$ - $b_3$  have m/z similar to that of standard. Increase in m/z was observed for  $a_4$ - $b_4$ ,  $a_5$ - $b_5$ ,  $a_6$ - $b_6$ ,  $a_7$ - $b_7$  and  $a_8$ - $b_8$ . This indicates that the possible modification is on base 3, (CCG\*CCCATG). This was further confirmed with  $w_n$  ions. Increase in m/z for  $w_7$  ion and all ions below  $w_6$  have m/z similar to that of standard. Table showing the m/z for standard and adducted Fragment 4 is as shown in Table S6.

**Table S6.** Calculated m/z for standard and singly adducted Fragment 4. (m/z highlighted in red were the ions with increased m/z compared to that of standard corresponding to BPDE adducted)

Fragment ion	m/z	
	Unadducted	Singly Adducted
$a_2$ - $b_2$	[466.1] <sup>-</sup>	[466.1] <sup>-</sup>
$a_3$ - $b_3$	[755.2] <sup>-</sup>	[755.2] <sup>-</sup>
$a_4$ - $b_4$	[1084.8] <sup>-</sup>	[1386.4] <sup>-</sup>
$a_5$ - $b_5$	[1373.8] <sup>-</sup>	[837.2] <sup>-2</sup>
$a_6$ - $b_6$	[1663.0] <sup>-</sup>	[981.8] <sup>-2</sup>
$a_7$ - $b_7$	[975.6] <sup>-2</sup>	[1126.3] <sup>-2</sup>
$a_8$ - $b_8$	[1132.2] <sup>-2</sup>	n/d
$w_2$	[650.2] <sup>-</sup>	[650.2] <sup>-</sup>
$w_3$	[963.3] <sup>-</sup>	[963.3] <sup>-</sup>
$w_4$	[1252.5] <sup>-</sup>	[1252.3] <sup>-</sup>
$w_5$	[1541.7] <sup>-</sup>	[770.2] <sup>-2</sup>
$w_6$	[915.1] <sup>-2</sup>	[914.8] <sup>-2</sup>
$w_7$	[1079.4] <sup>-2</sup>	[1230.9] <sup>-2</sup>



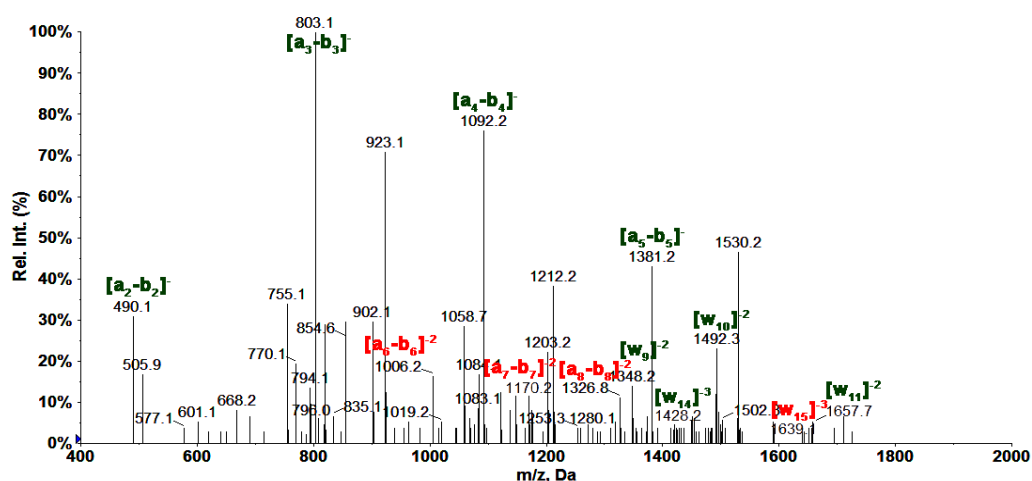
**Figure S7.** LC-MS of ds-32 bp exon 7 probe: (A) Extracted ion chromatogram of singly adducted Fragment 3, m/z 1234.4 (B) MSMS spectra of fragment ion m/z, 1234.4 showing the obtained  $a_n$ - $b_n$  and  $w_n$  ions. Ions with m/z similar to standard are shown in green and ions with increased m/z shown in red



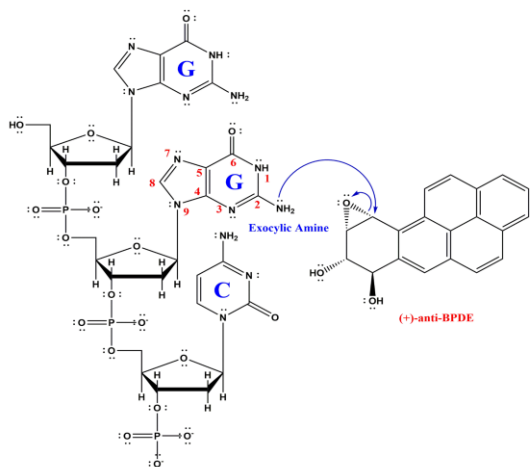
Singly adducted Fragment 3 has an m/z of 1234.4 with a charge of -6. Extracted ion chromatogram of 1234.4 is as shown in Figure S8A. XIC of 1012.6 show one major peak indicating that there is one major adduct on Fragment 3. MSMS spectra for singly adducted Fragment 3, m/z 1234.4 is as shown in Figure S8B. All a<sub>n</sub>-b<sub>n</sub> ions up to a<sub>5</sub>-b<sub>5</sub> have m/z similar to that of standard. Increase in m/z was observed for a<sub>6</sub>-b<sub>6</sub>, a<sub>7</sub>-b<sub>7</sub> and a<sub>8</sub>-b<sub>8</sub> and w<sub>19</sub>. This indicates that the possible modification is on base 5, (TGAGG\*ATGGGCCTCCGGTTCATG). Table showing the m/z for standard and adducted Fragment 4 is as shown in Table S7.

**Table S7.** Calculated m/z for standard and singly adducted DNA fragments of fragment 3. (m/z highlighted in red were the ions with increased m/z compared to that of standard corresponding to BPDE adducted)

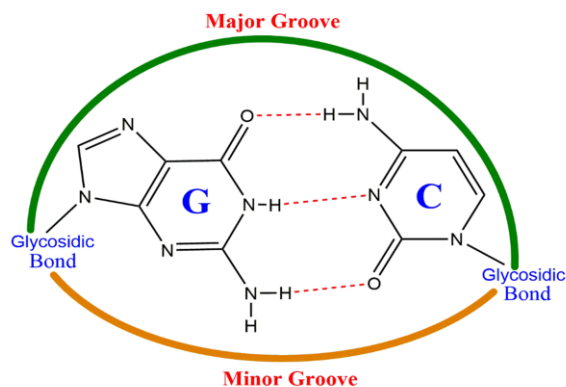
Fragment ion	m/z	
	Unadducted	Singly Adducted Fragment
a <sub>2</sub> -b <sub>2</sub>	[401.1] <sup>-</sup>	[401.1] <sup>-</sup>
a <sub>3</sub> -b <sub>3</sub>	[730.2] <sup>-</sup>	[730.2] <sup>-</sup>
a <sub>4</sub> -b <sub>4</sub>	[1043.3] <sup>-</sup>	[1043.3] <sup>-</sup>
a <sub>5</sub> -b <sub>5</sub>	[1372.4] <sup>-</sup>	[1372.4] <sup>-</sup>
a <sub>6</sub> -b <sub>6</sub>	[1702.0] <sup>-</sup>	[1001.3] <sup>-2</sup>
a <sub>7</sub> -b <sub>7</sub>	[1007.2] <sup>-2</sup>	[1158.8] <sup>-2</sup>
a <sub>8</sub> -b <sub>8</sub>	n/d	[1309.9] <sup>-2</sup>
a <sub>9</sub> -b <sub>9</sub>	[1323.8] <sup>-2</sup>	[1474.9] <sup>-2</sup>
w <sub>17</sub>	[1755.6] <sup>-3</sup>	n/d
w <sub>18</sub>	[1395.6] <sup>-3</sup>	n/d
w <sub>19</sub>	[1477.9] <sup>-4</sup>	[1242.7] <sup>-5</sup>
w <sub>20</sub>	[1541.7] <sup>-</sup>	n/d
w <sub>21</sub>	[915.1] <sup>-2</sup>	n/d



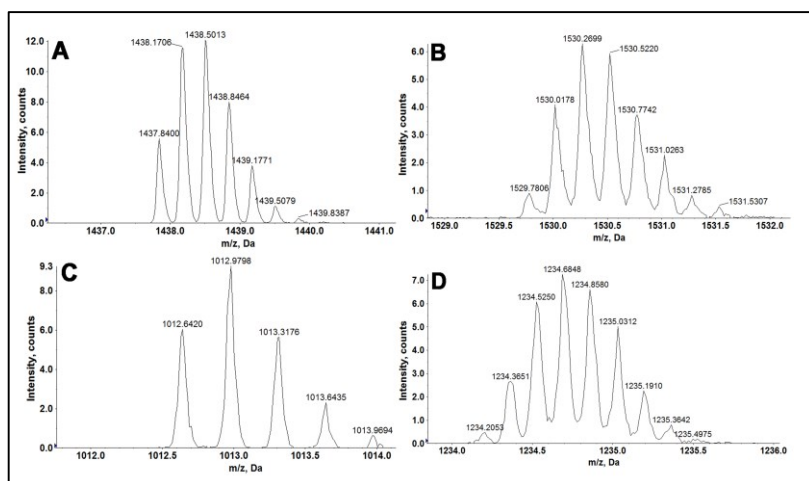
**Figure S8.** LC-MS of ds-32 bp exon 7 probe: MS/MS spectrum of 1530.3 showing a<sub>n</sub>-b<sub>n</sub> and w<sub>n</sub> ions. Ions with m/z similar to standard labeled in green and ions with increased m/z in red in 10mM Tris buffer, pH 7.4 and 0.1M NaCl.



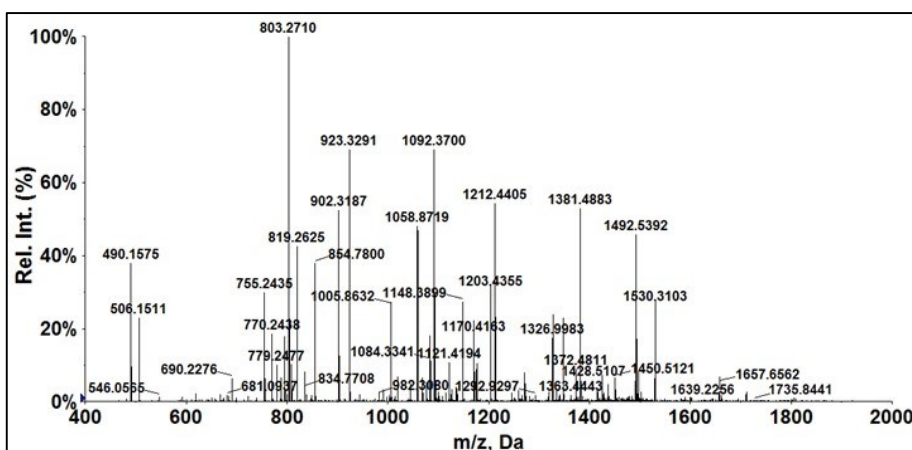
**Scheme S2.** Chemical structure of sequence GGC. Numbering of guanine shown in red. Proposed mechanism for attack of BPDE on exocyclic amine of guanine of DNA.



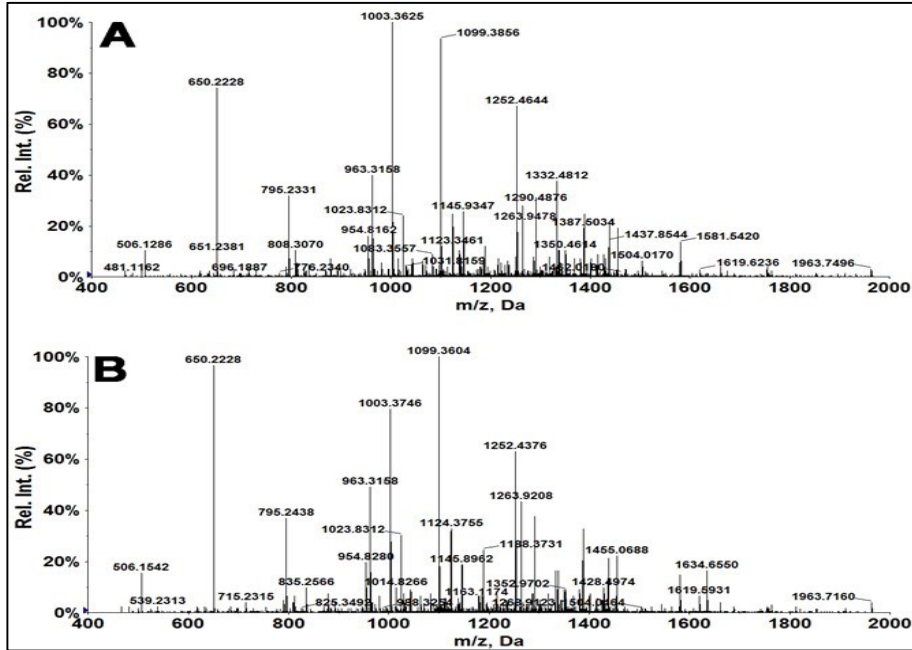
**Scheme S3.** Minor groove and Major groove of GC base pair of duplex DNA.



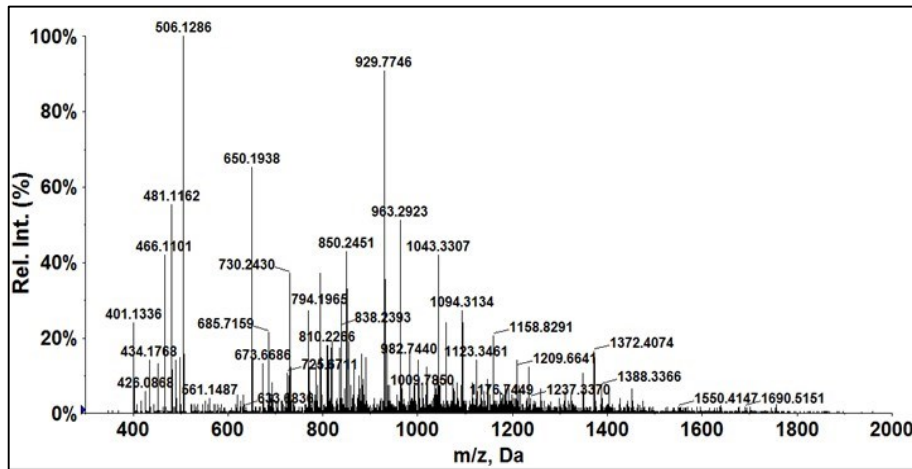
**Figure S9.** Representation of isotopic distribution ds DNA exon 7 probe for obtained ions A) Fragment 1, m/z 1437.8 (-3), B) Fragment 2, m/z 1530.3 (-3) C) Fragment 3, m/z 1012.6 (-3) D) Fragment 4, m/z 1234.4 (-6), measured on a Qstar Elite mass spectrometer (Sciex, USA)



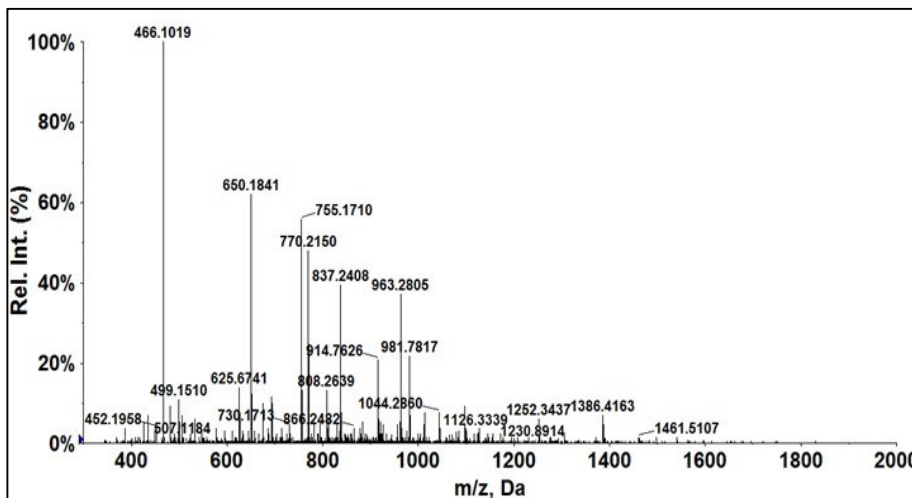
**Figure S10.** LC-MS/MS of ds-32 bp exon 7 probe: Raw data of ToF MS/MS images for Fragment 2.



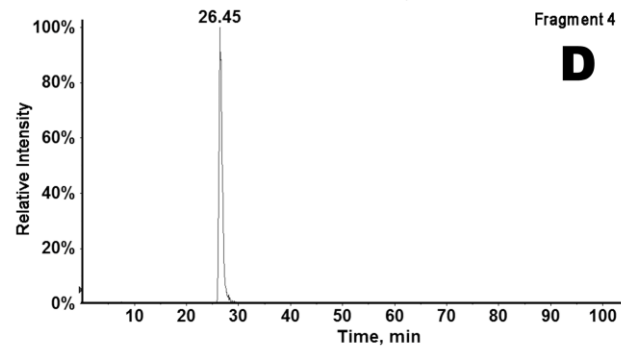
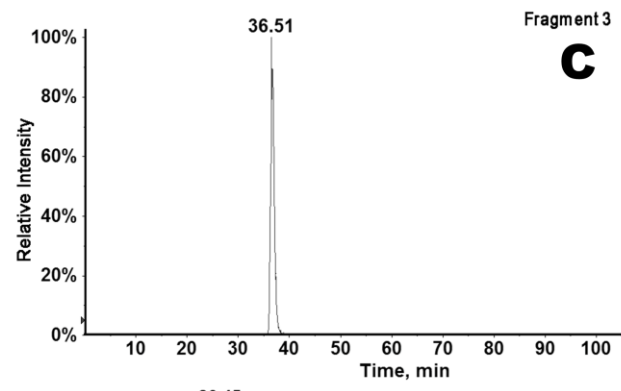
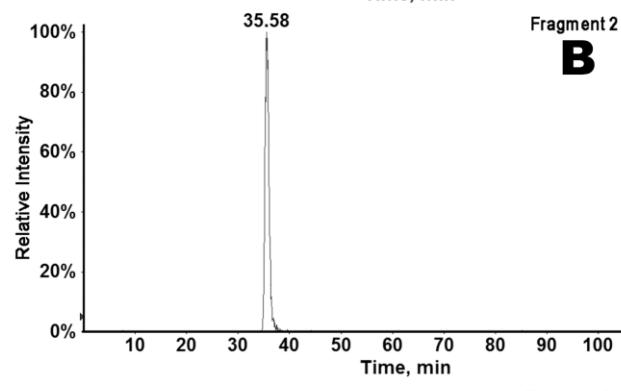
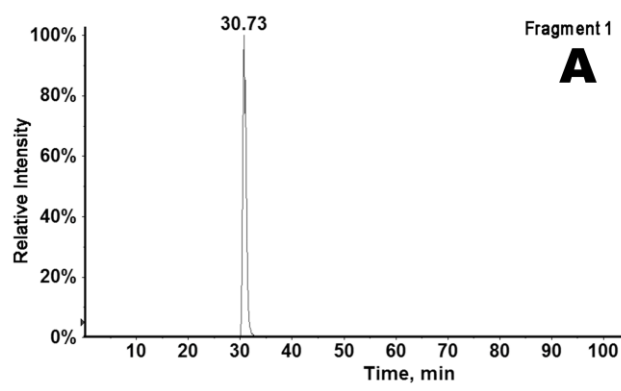
**Figure S11.** LC-MS/MS of ds-32 bp exon 7 probe: Raw data of ToF MS/MS images for Fragment 1 A) Peak 1 B) Peak 2.



**Figure S12.** LC-MS/MS of ds-32 bp exon 7 probe: Raw data of ToF MS/MS images for Fragment 3.



**Figure S13.** LC-MS/MS of ds-32 bp exon 7 probe: Raw data of ToF MS/MS images for Fragment 4.



**Figure S14.** Extracted ion chromatogram of standard unadducted fragments of 32 bp ds DNA after NlaIII treatment. (A) XIC of Fragment-1, 13 mer m/z, 1337.5 charge -3. (B) XIC of Fragment-2, 19 mer, m/z 1454.6 charge -4 (C) XIC of Fragment-3, 23 mer m/z 1421.3 charge -5 (D) XIC of Fragment-4, 9 mer m/z 912.2 charge -3.