

Supporting Information for

**“Recognition and Incision of Oxidative Intrastrand Cross-link Lesions by
UvrABC Nuclease”**

by

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Figure S1. ESI-MS of the starting materials: (A) d(GTAG^{Br}CAT); (B) d(ATGGCG^{PhSm}CGCTAT); (c) d(ATGGCG^{PhSm}UGCTAT).

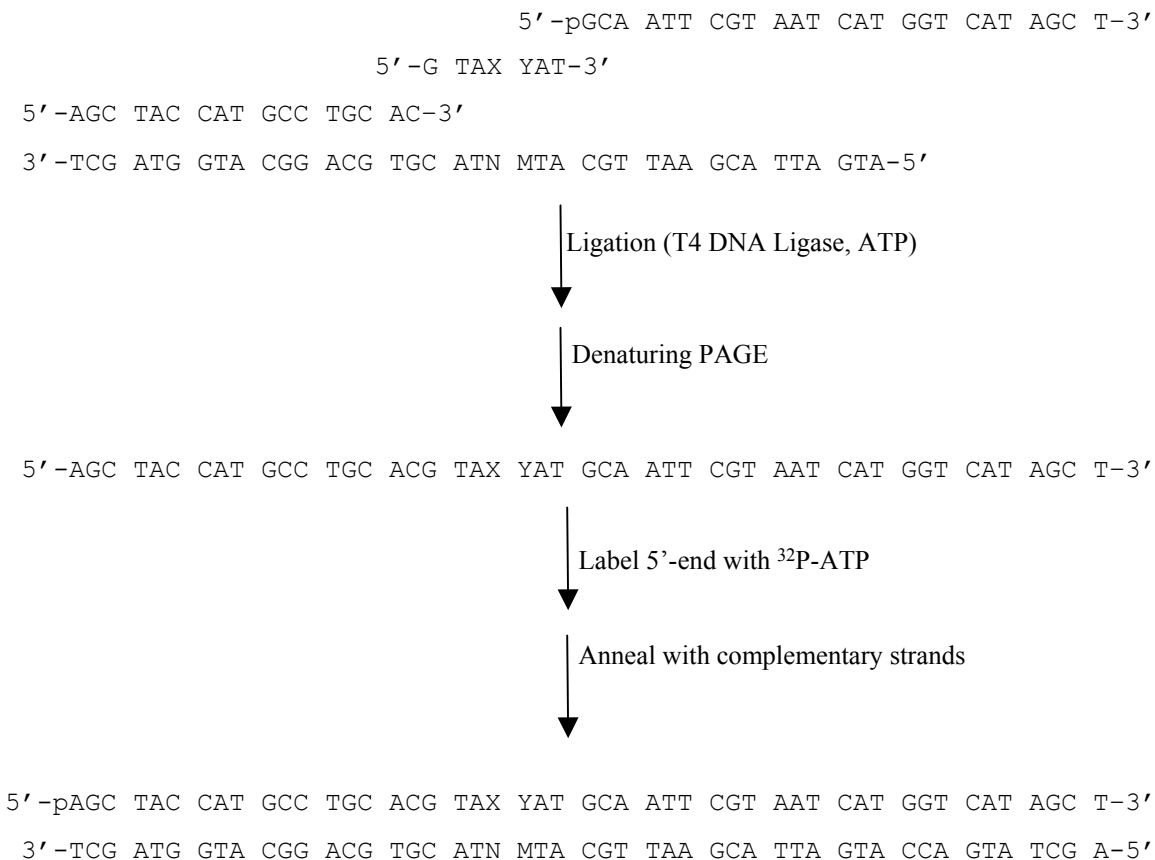
Figure S2. HPLC trace for the separation of the UVC irradiation mixture of single-stranded d(GTATTAT).

Figure S3. Isolation and characterization of d(GTAG[8-5]CAT). (A) HPLC trace for the separation of the 310-nm irradiation mixture of d(GTAG^{Br}CAT) with TEAA buffer. (B) HPLC trace for the re-separation of d(GTAG[8-5]CAT) with phosphate buffer. (C) Negative-ion ESI-MS of d(GTAG[8-5]CAT). (C) Product-ion spectrum of the ESI-produced [M-3H]³⁻ ion (*m/z* 1058.0) of d(GTAG[8-5]CAT).

Figure S4. Isolation and characterization of d(ATGGCG[8-5m]CGCTAT). (A) HPLC trace for the separation of the 254-nm irradiation mixture of d(ATGGCG^{PhSm}CGCTAT). (B) Negative-ion ESI-MS of d(ATGGCG[8-5m]mCGCTAT). (C) Product-ion spectrum of the ESI-produced [M-3H]³⁻ ion (*m/z* 1223.0) of d(ATGGCG[8-5m]mCGCTAT).

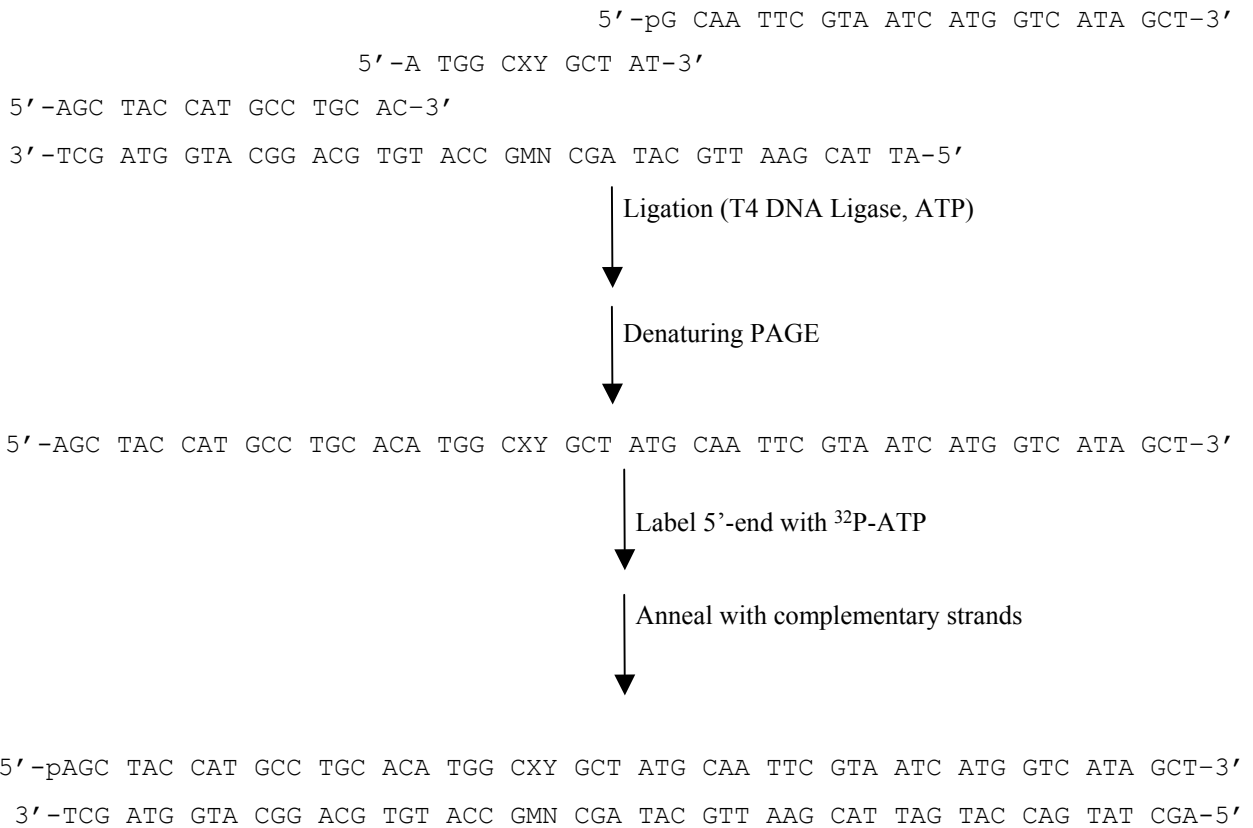
Figure S5. Isolation and characterization of d(ATGGCG[8-5m]TGCTAT). (A) HPLC trace for the separation of the 254-nm irradiation mixture of d(ATGGCG^{PhSm}UGCTAT) with TEAA buffer. (B) HPLC trace for the re-separation of d(ATGGCG[8-5m]TGCTAT) with phosphate buffer. (C) Negative-ion ESI-MS of d(ATGGCG[8-5m]TGCTAT). (D) Product-ion spectrum of the ESI-produced [M-3H]³⁻ ion (*m/z* 1223.0) of d(ATGGCG[8-5m]TGCTAT)

Figure S6. Non-linear regression analysis of the plot of average percentage binding (determined from EMSA with three or more sets of titrations per duplex) versus the concentrations of UvrA for duplexes containing: (A) G[8-5]C-54bp; (B) G[8-5m]mC-54bp; (C) G[8-5m]T-54bp.



Sequence	XY•MN	Ligation Yield (%)
T[c,s]T-49bp	T[c,s]T•AA	25
T[6-4]T-49bp	T[6-4]T•AA	5
G[8-5]C-49bp	G[8-5]C•GC	12

Scheme S1. (Nucleobases X and Y or M and N of each strand are listed, and both of them are in the 5'-to 3'- sequence order.)



Sequence	XY•MN	Ligation Yield (%)
G[8-5]T-54bp	G[8-5]C•GC	21
G[8-5m]mC-54bp	G[8-5m]mC•GC	17
G[8-5m]T-54bp	G[8-5m]T•AC	10

Scheme S2. (Nucleobases X and Y or M and N of each strand are listed, and both of them are in the 5'-to 3'- sequence order.)

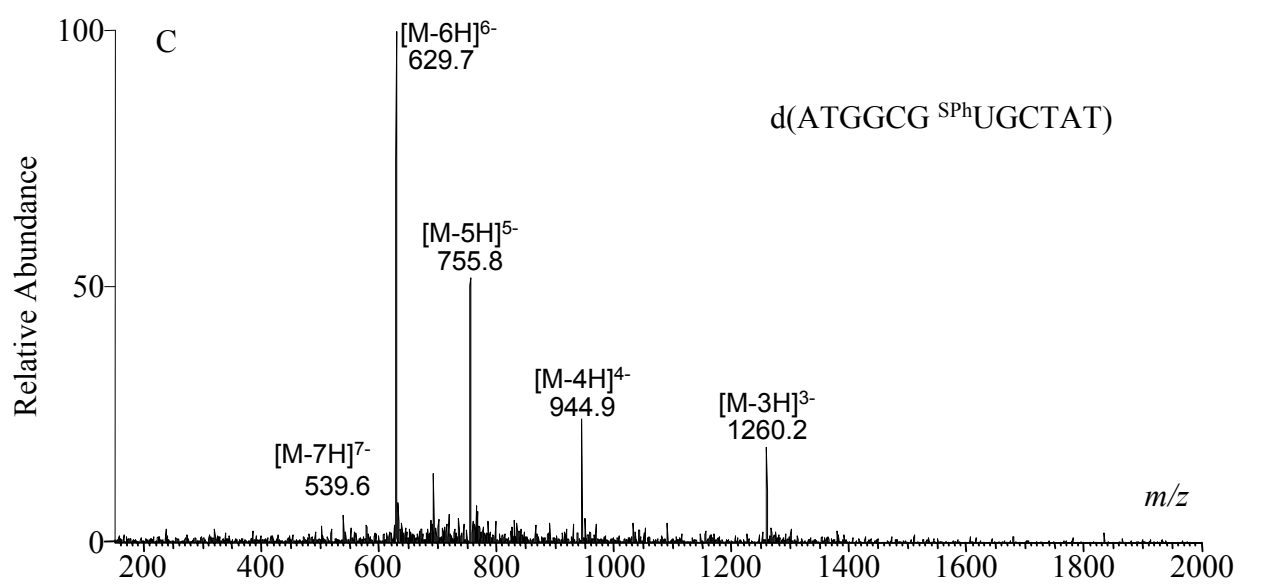
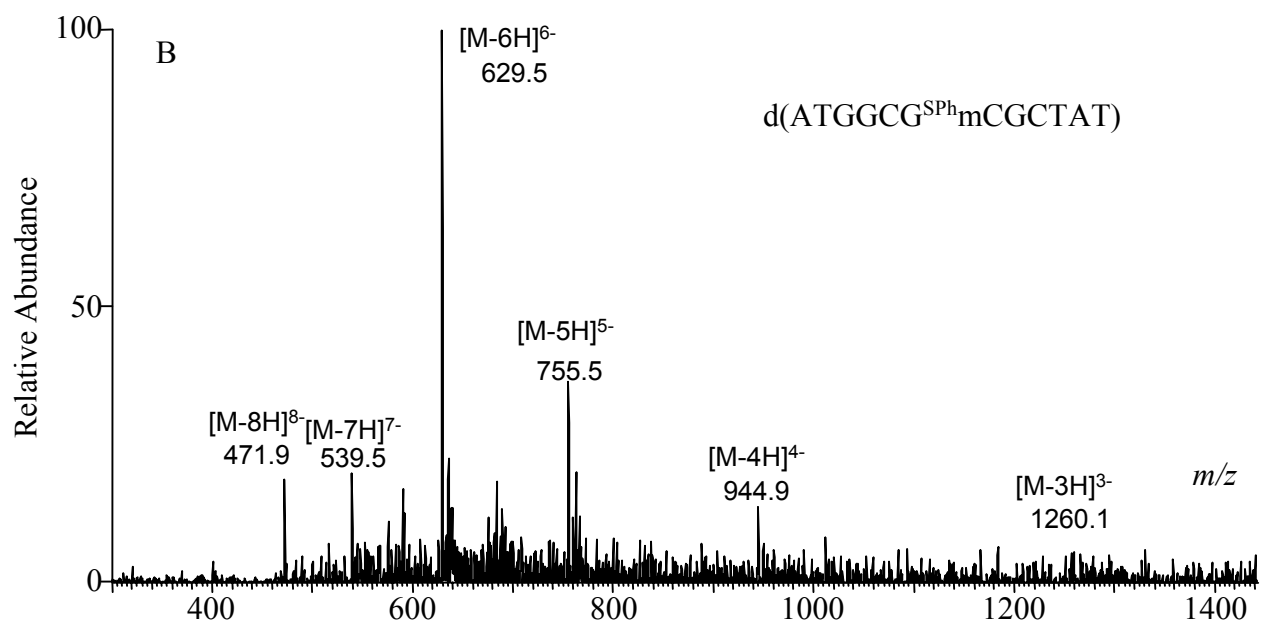
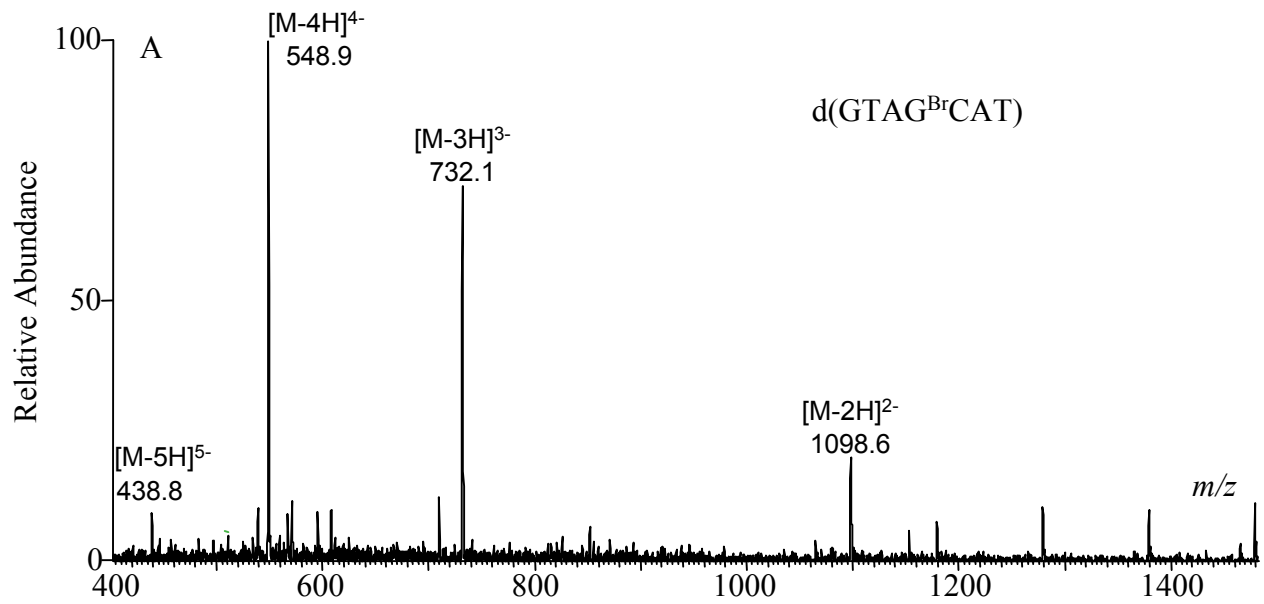


Figure S1.

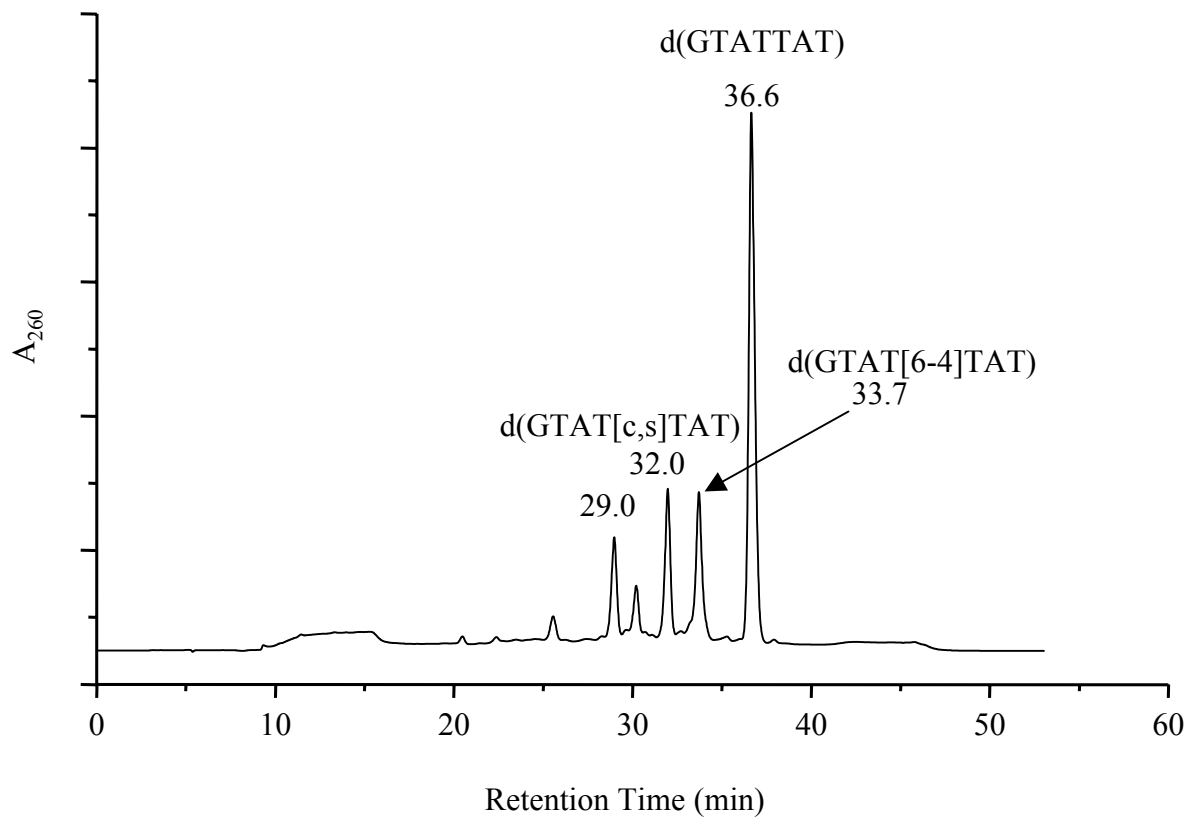
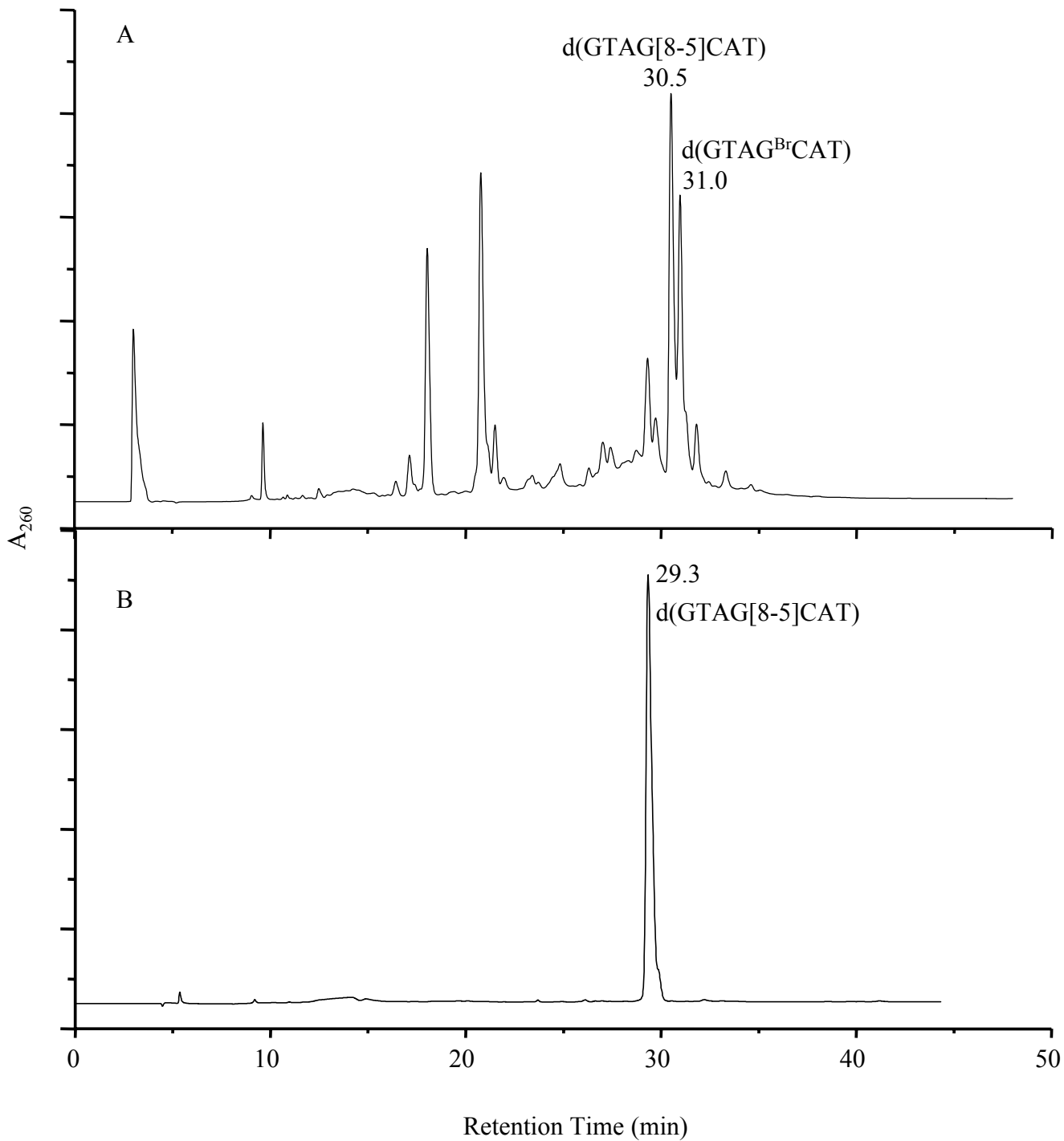


Figure S2.



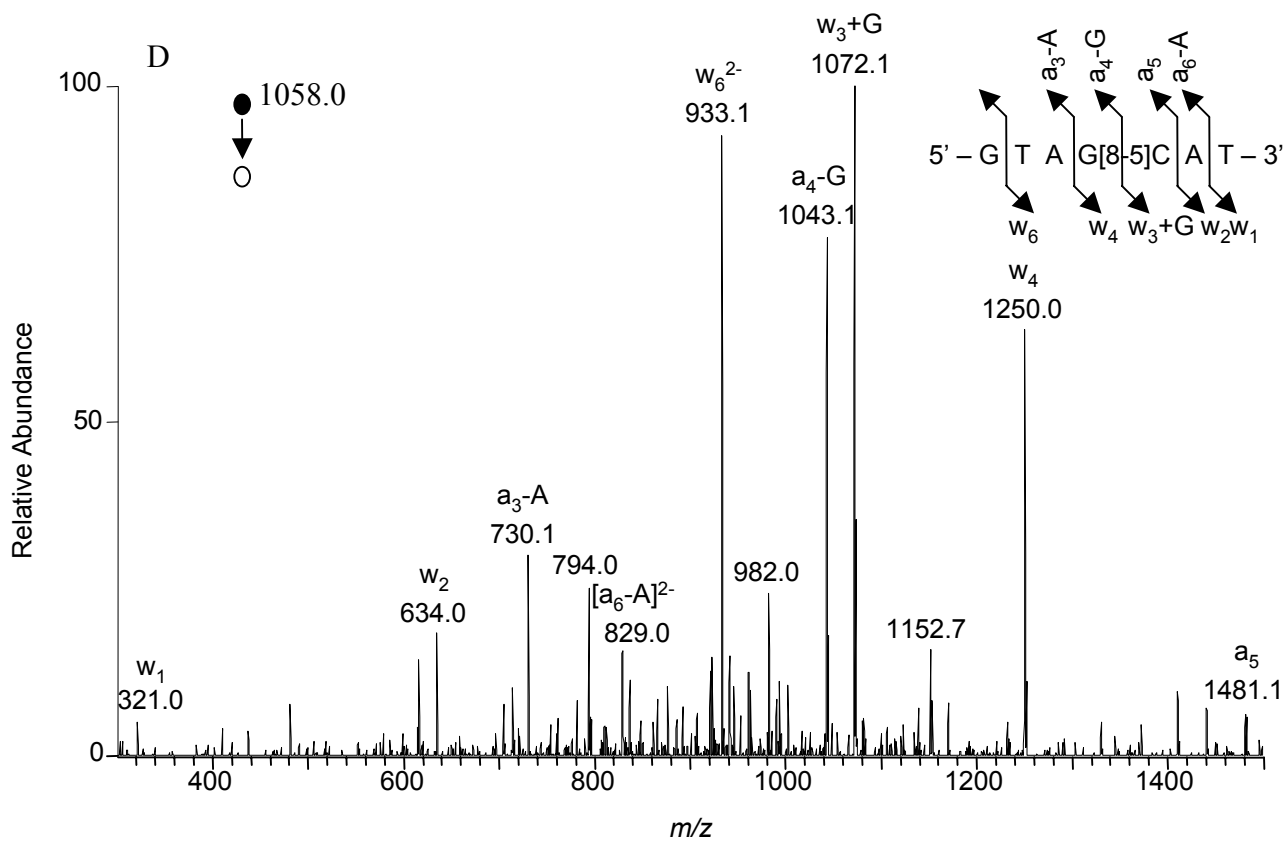
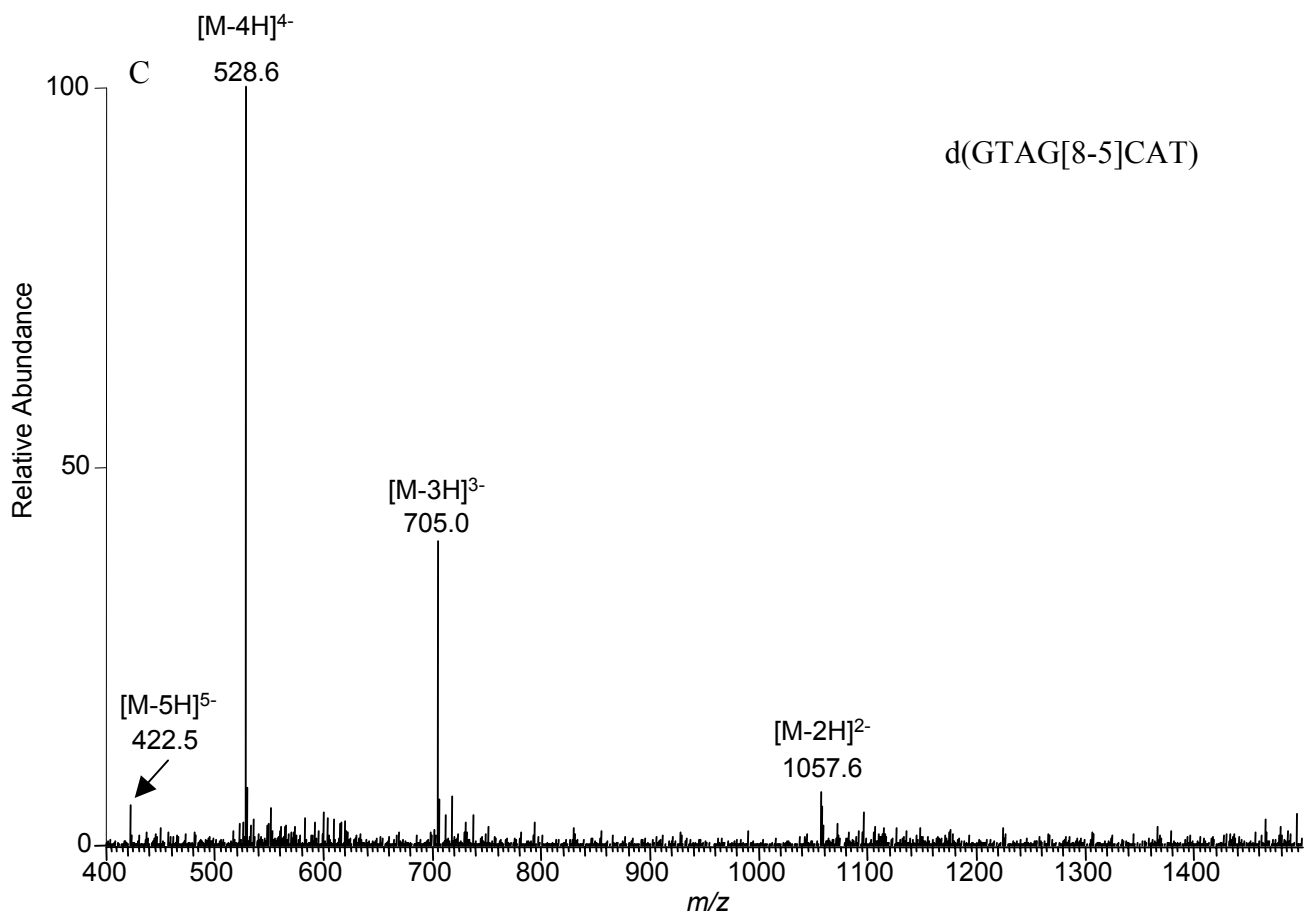
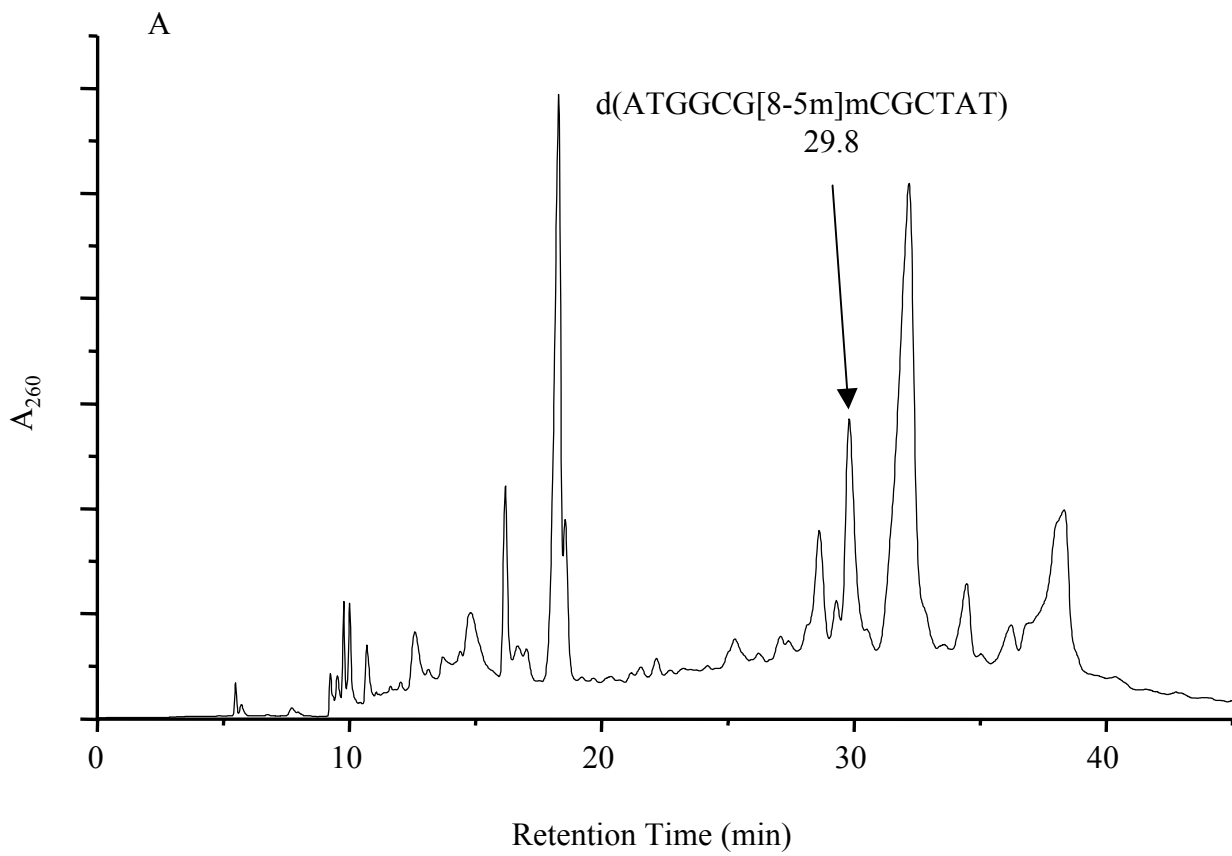


Figure S3.



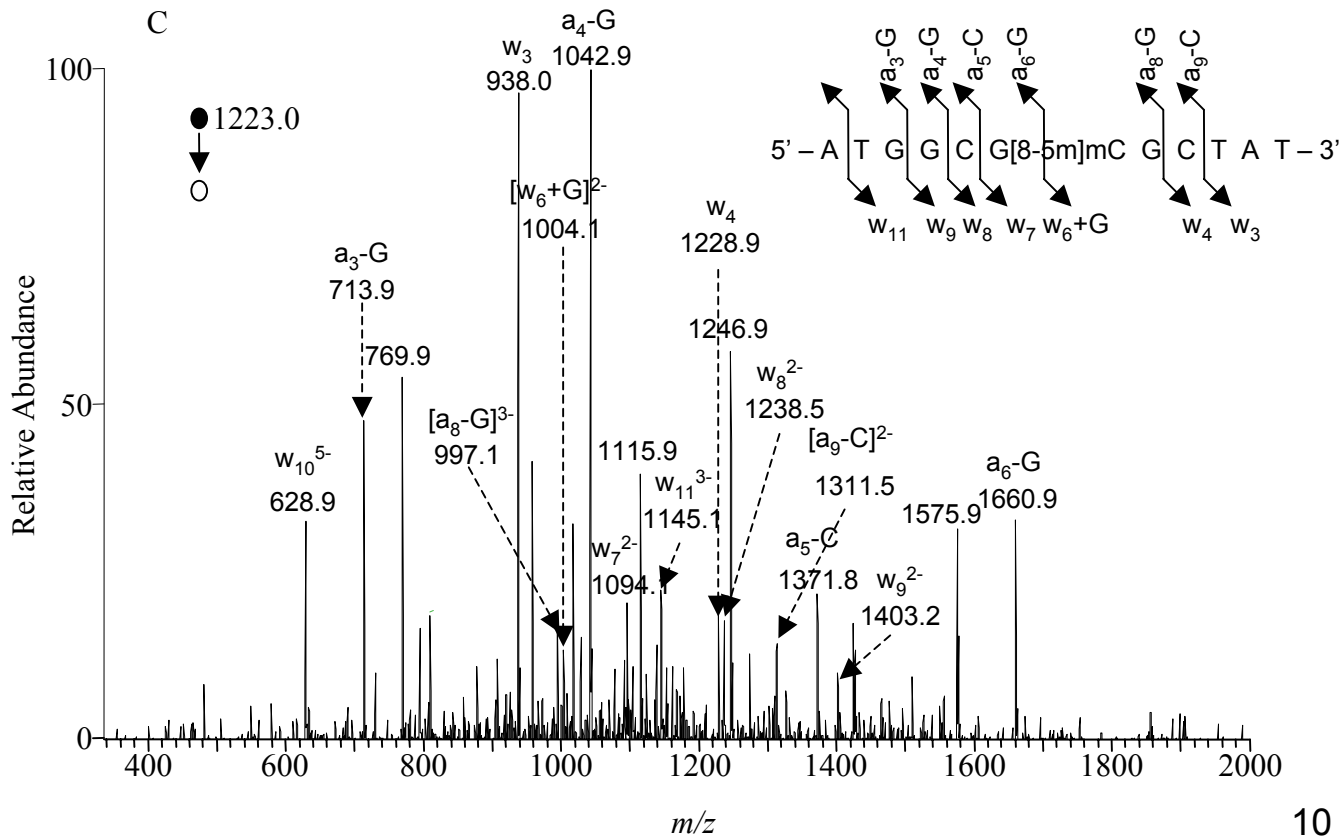
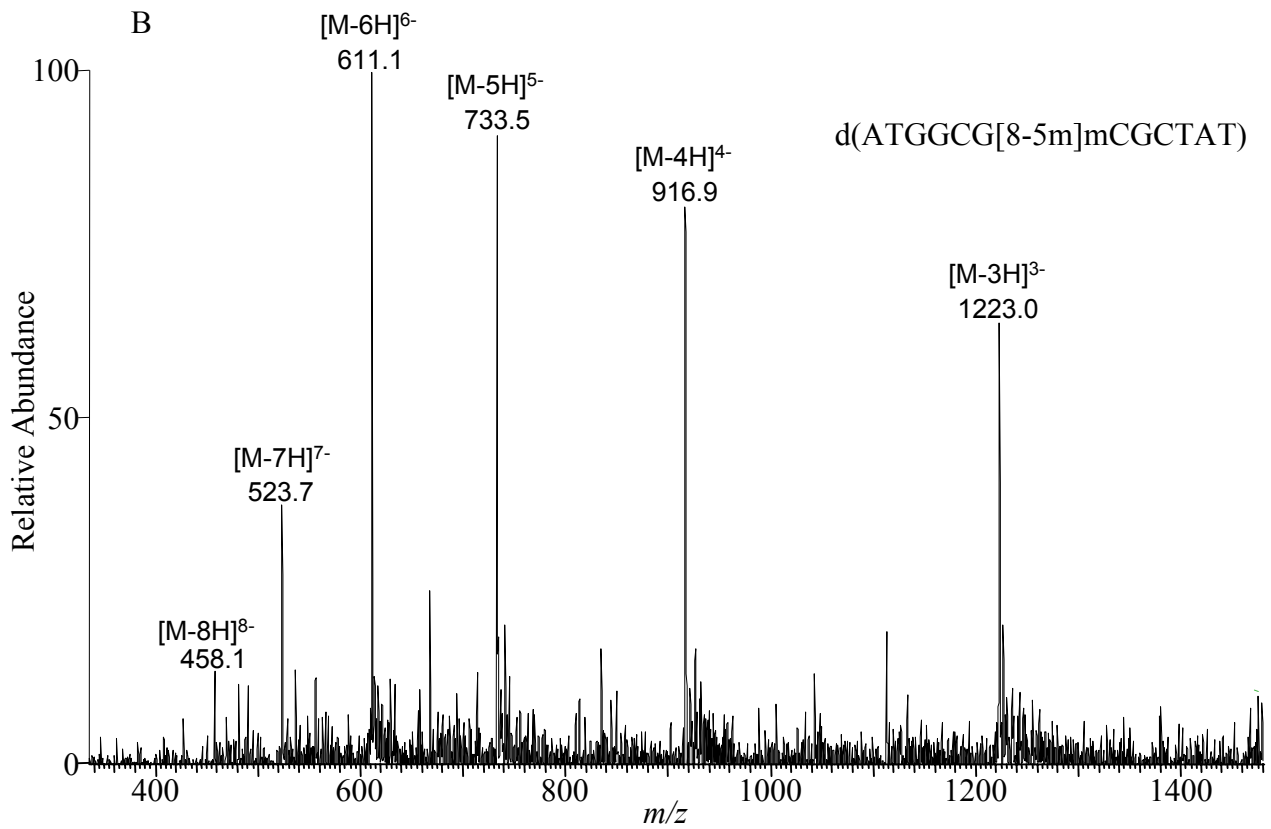
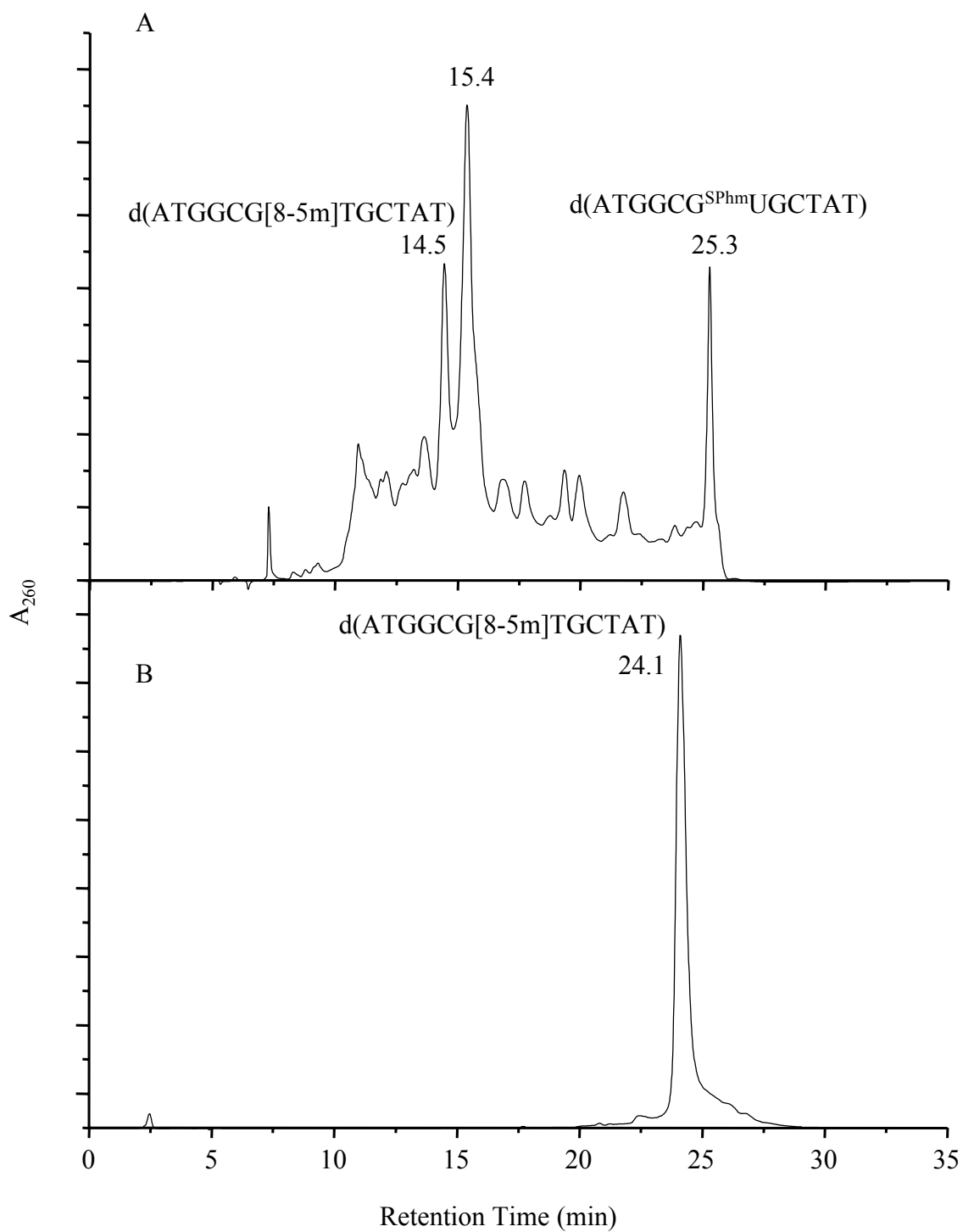


Figure S4.



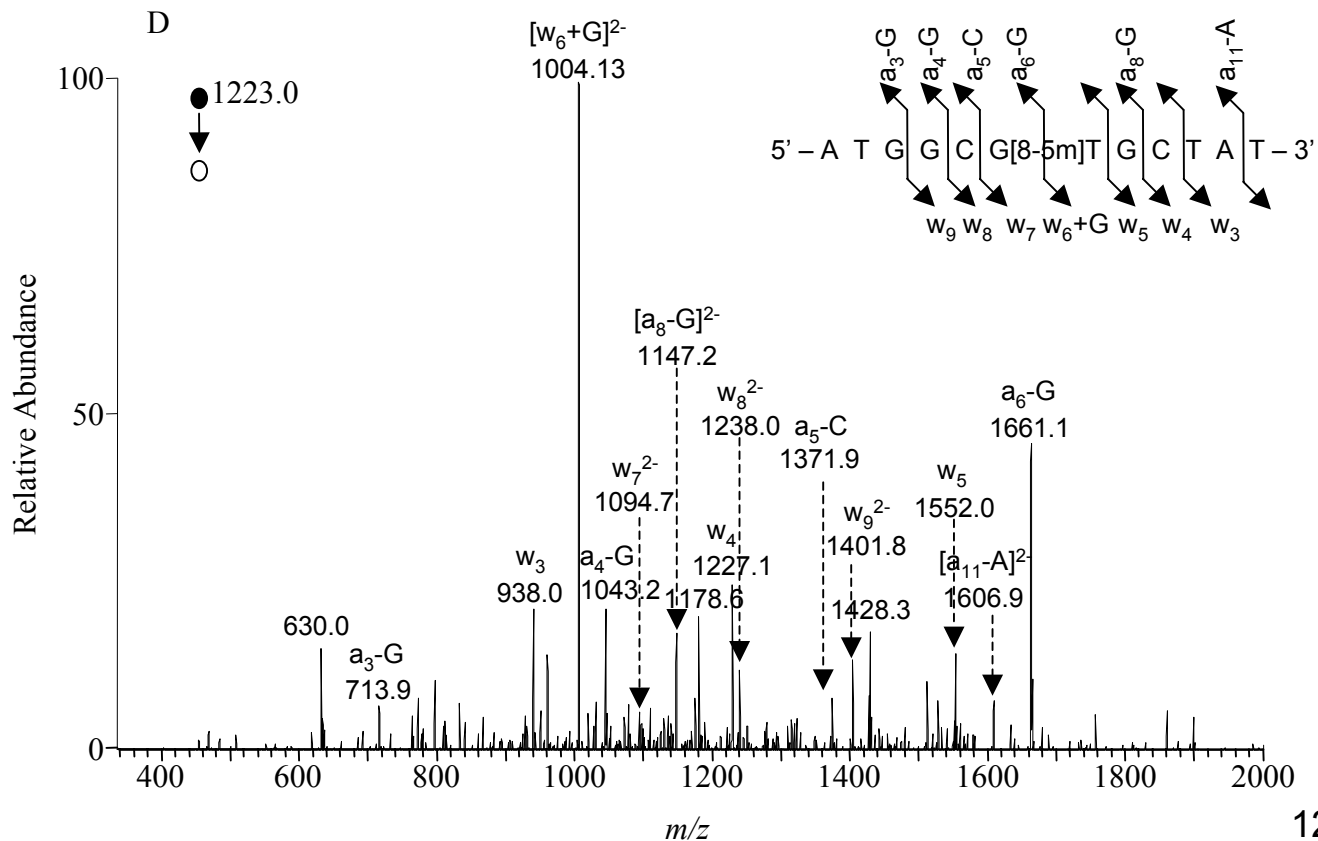
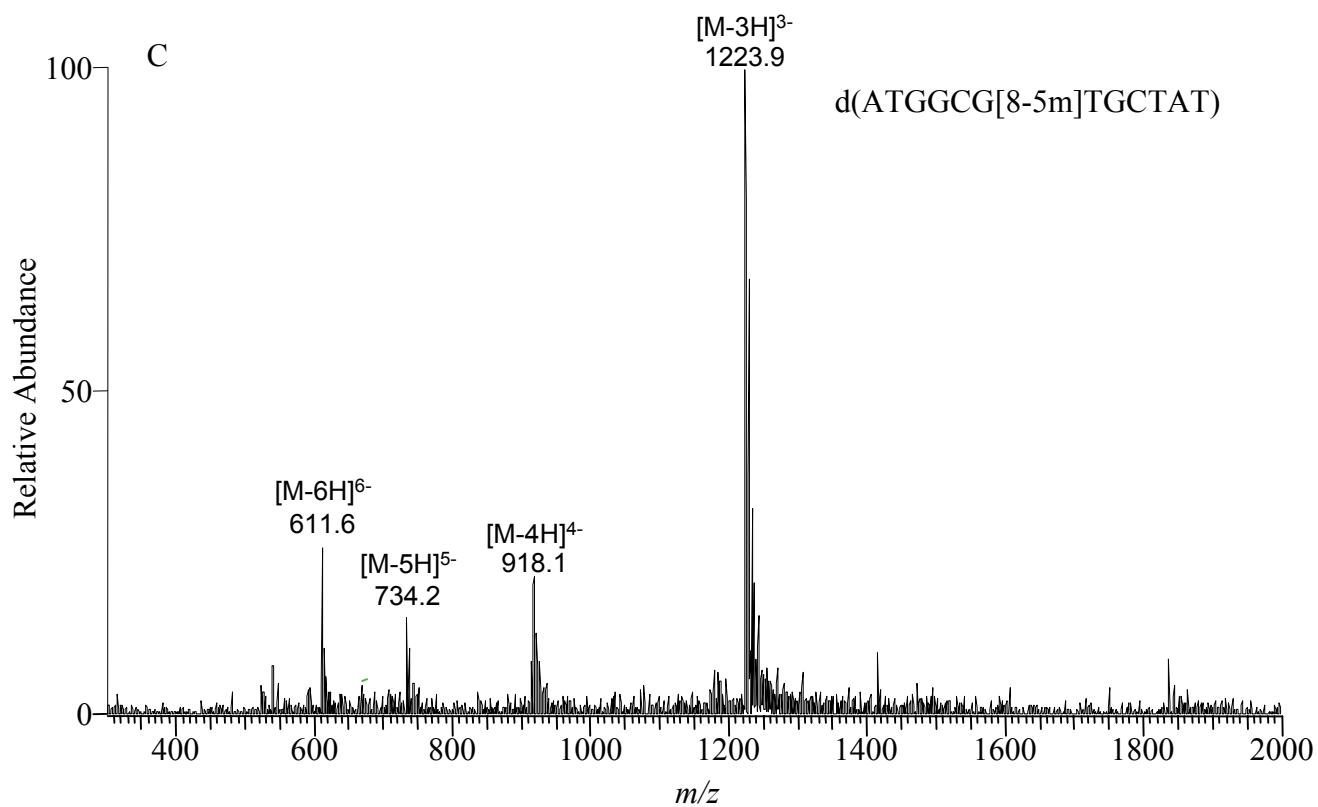


Figure S5.

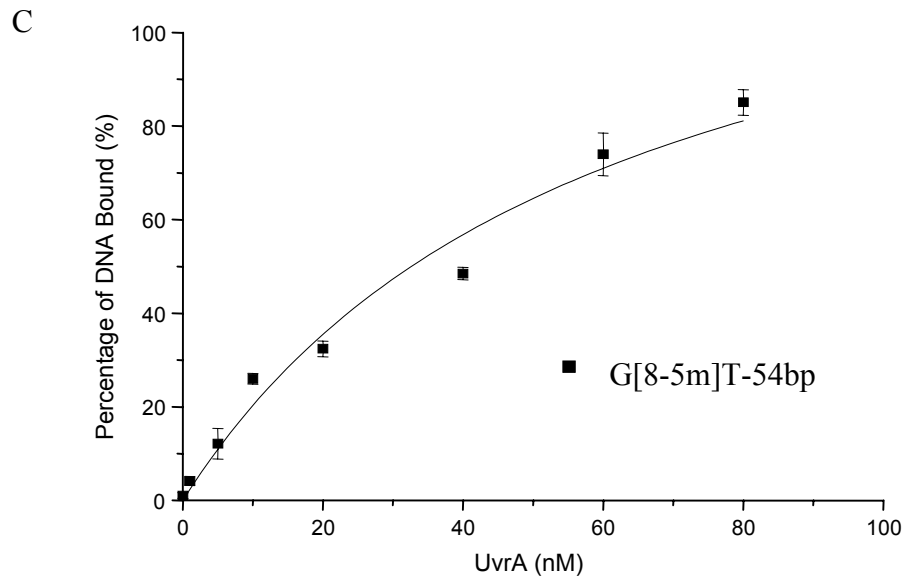
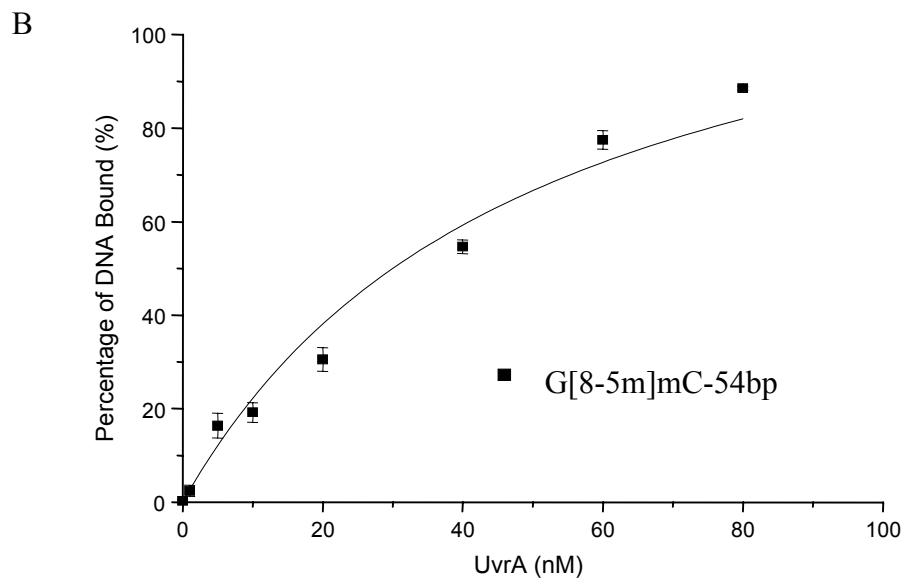
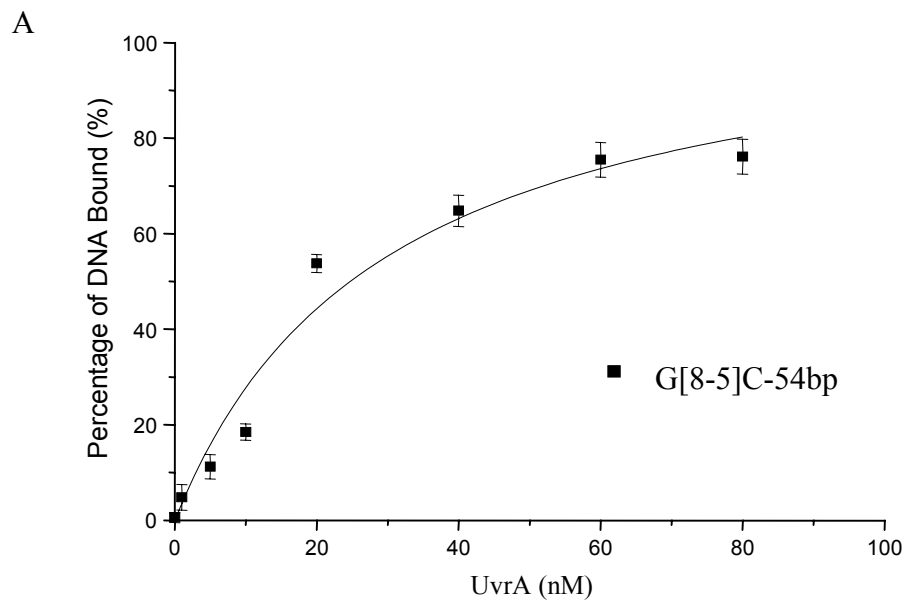


Figure S6.