Electronic Supplementary Material

Facile Formation of a DNA Adduct of Semicarbazide on Reaction with Apurinic/Apyrimidinic Sites in DNA

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CONTENT

6. **Figure S6** Analysis of the kinetic data for reaction of SEM with single- and double- stranded oligonucleotide DNA. Data were fitted linearly in the graphs.

7. **Figure S7** Method validation with synthesized SEM-tagged, AP site-containing oligodeoxynucleotides. The concentration of SEM-dR adduct measured by the developed LC-MS/MS method was directly proportional to the concentration of the oligodeoxynucleotides spiked to the cells. The data represent mean ± SD for three independent experiments

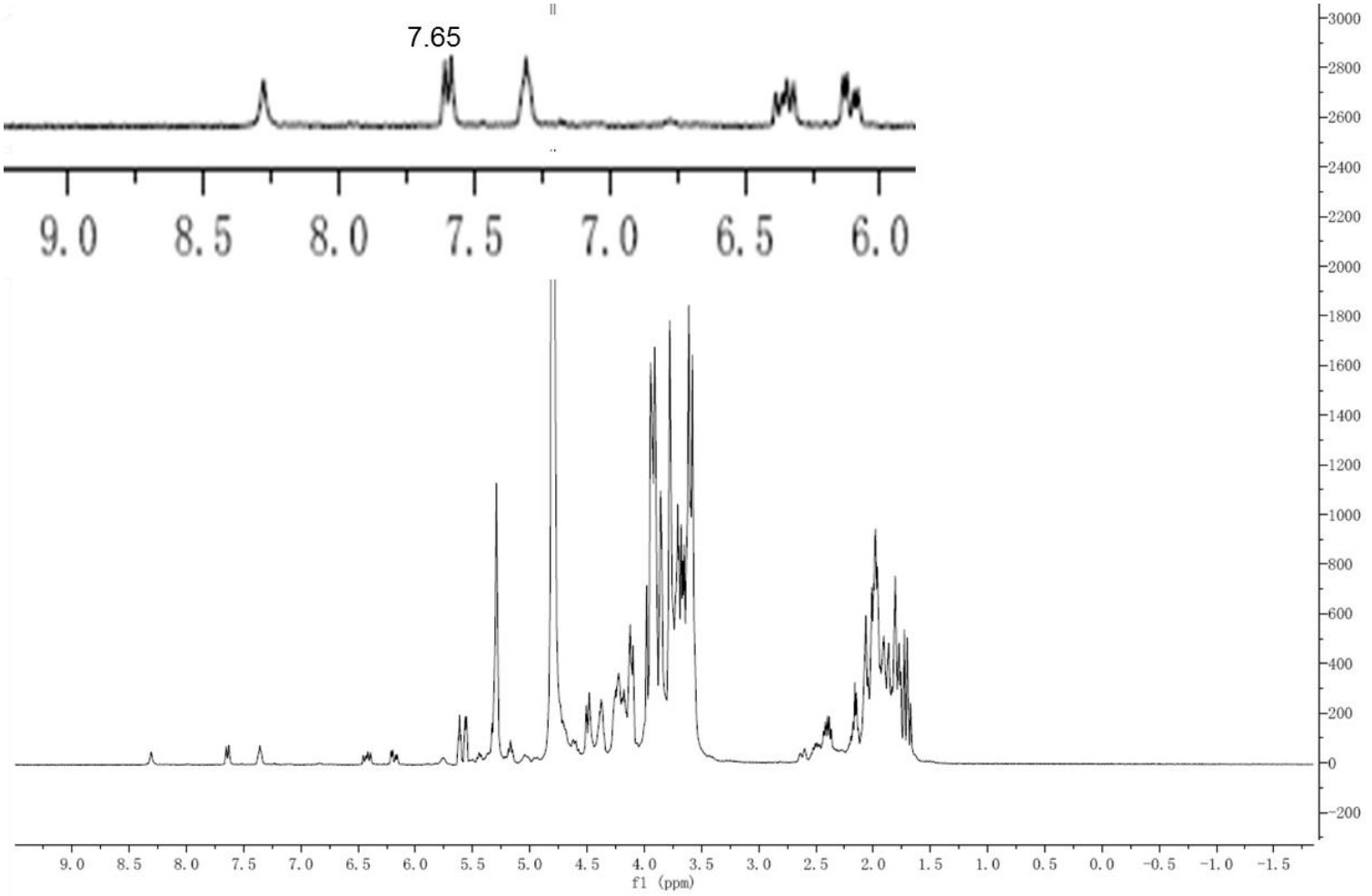

Figure S1 NMR spectrum from 1H NMR analysis of the adduct formed by reacting SEM with 2'-deoxyribose.

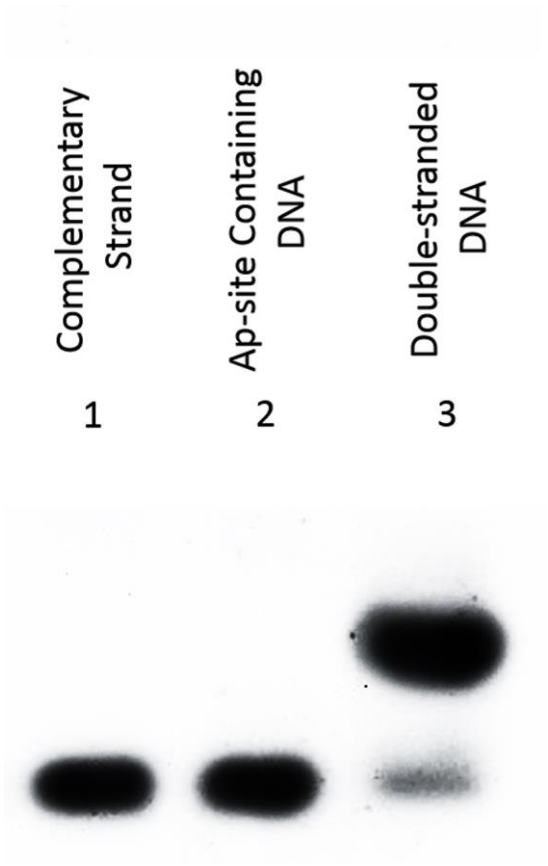

Figure S2 Gel electrophoresis analysis of the single- and double stranded oligonucleotides. Efficient formation of duplex AP site-containing DNA was observed as the AP site-containing oligonucleotide was annealed with 1.2 X molar excess of its complementary strand DNA.

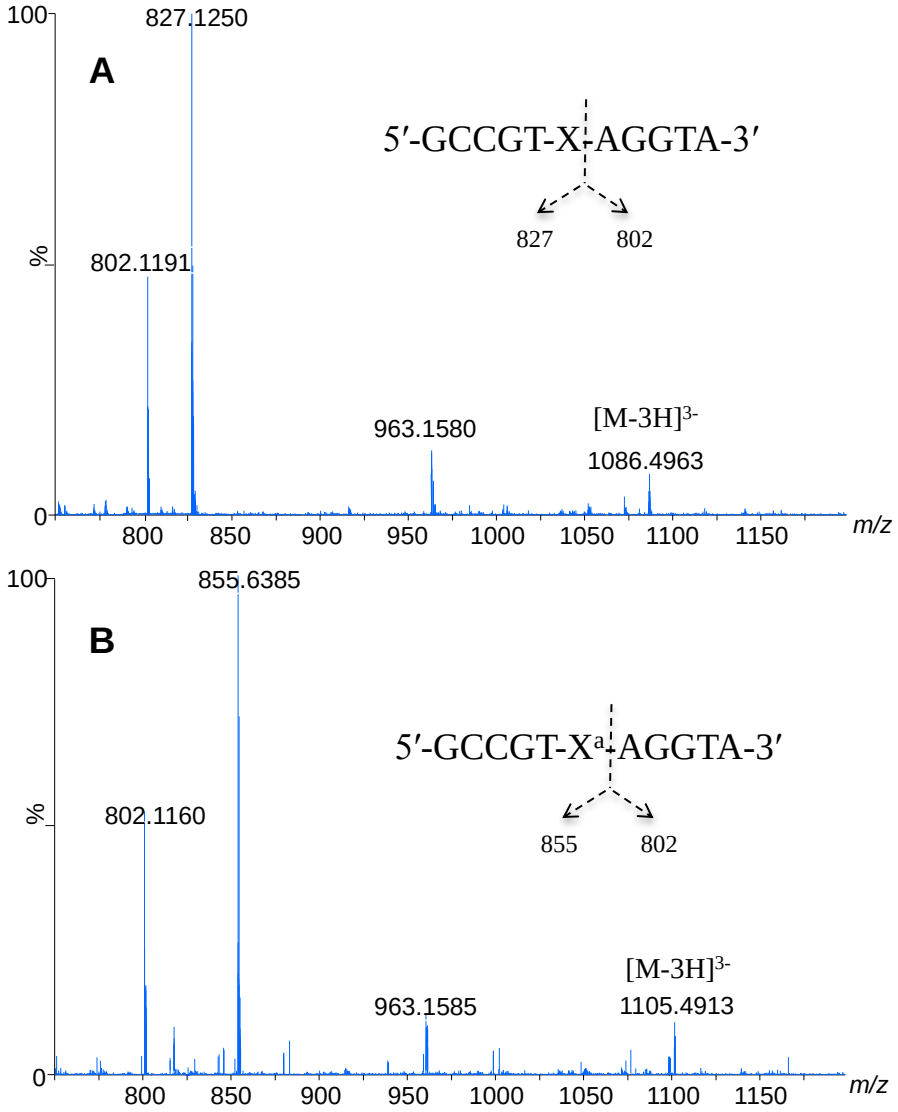

Figure S3 Product ion spectra of the $[M-3H]^{3-}$ ions of (A) AP site-containing oligonucleotide and (B) its SEM adduct. X and X^a indicate AP site and its SEM adduct, respectively. Fragment ions were observed as doubly charged state in the negative ESI-MS/MS analysis.

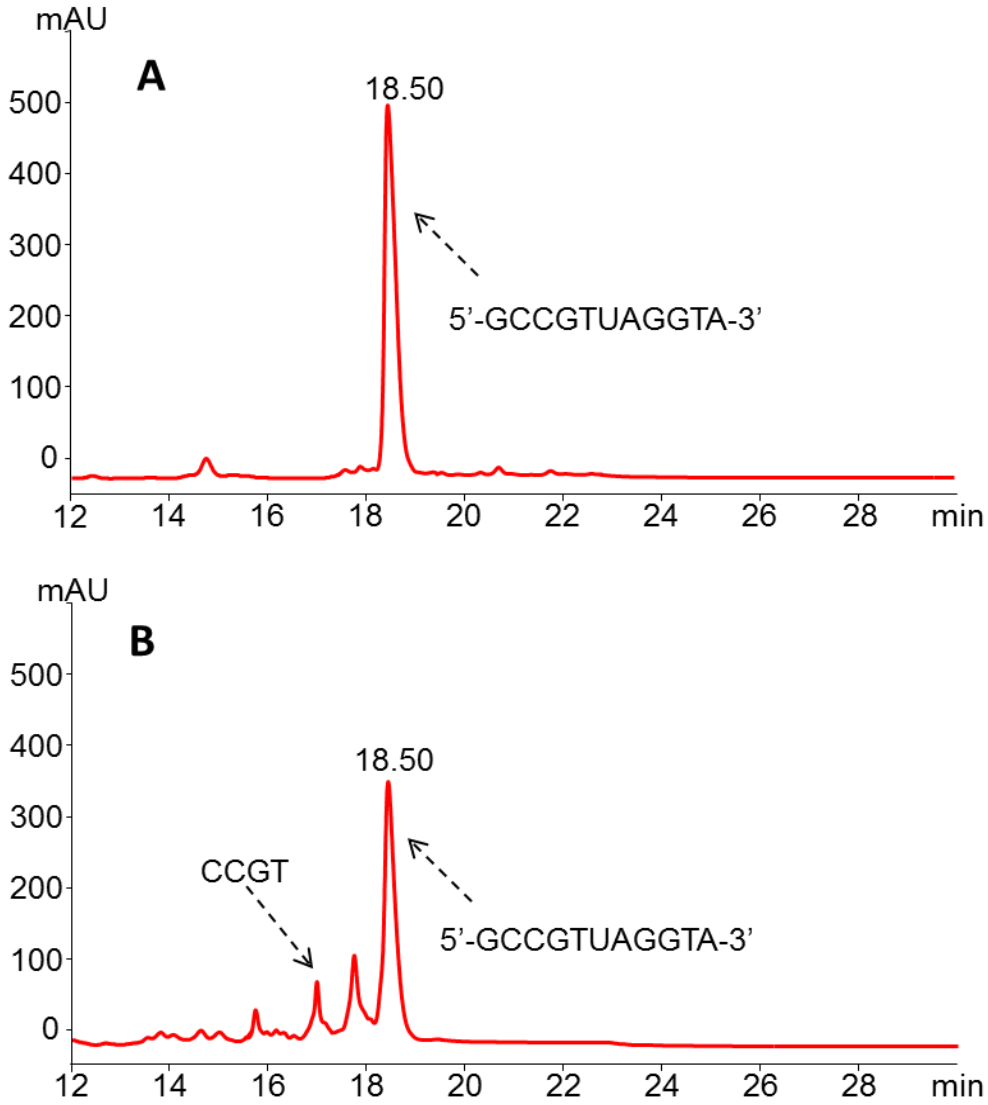

Figure S4 DNA oligonucleotide (A) before and (B) after overnight reaction with SEM in pH 3.5 at 37 °C.

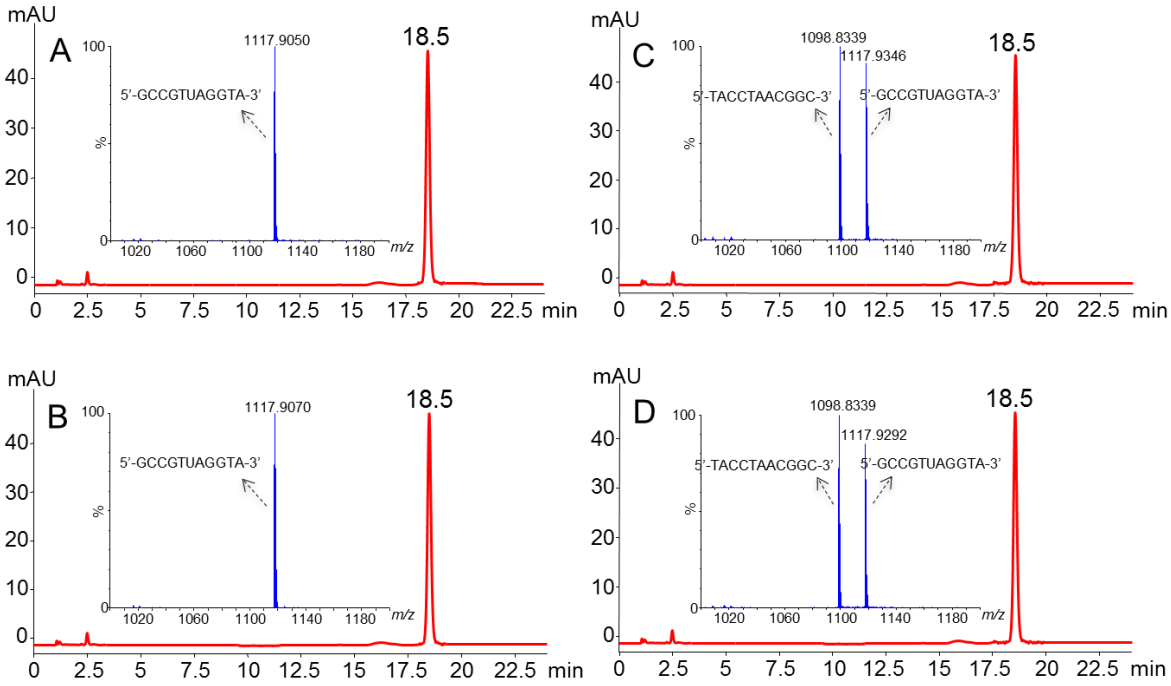

Figure S5 HPLC analyses of single-stranded (A and B) and double-stranded oligonucleotides (C and D) that do not contain abasic sites; in before (A and C) and after (B and D) reacting with SEM. Shown in the insets are the ESI-MS spectrum from Q-TOF MS analysis of the collected HPLC fraction containing the oligonucleotides. No cytosine adduct formation was observed in both the HPLC and ESI-MS analyses.

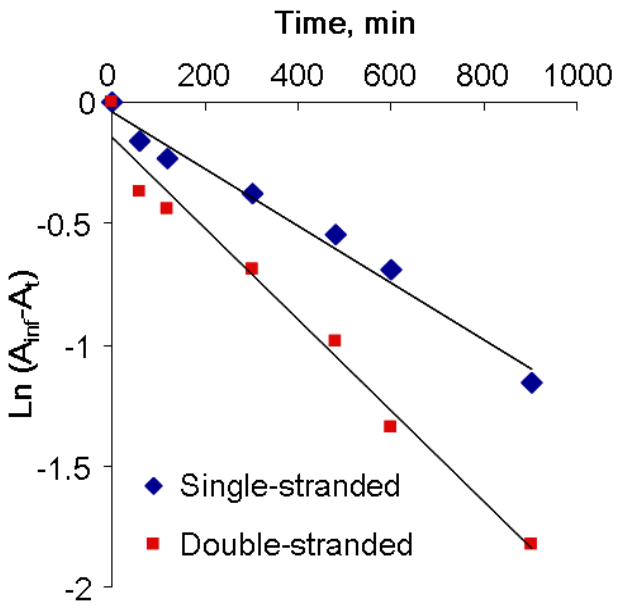

Figure S6 Analysis of the kinetic data for reaction of SEM with single- and double-stranded oligonucleotide DNA. Data are fitted linearly in the graphs.

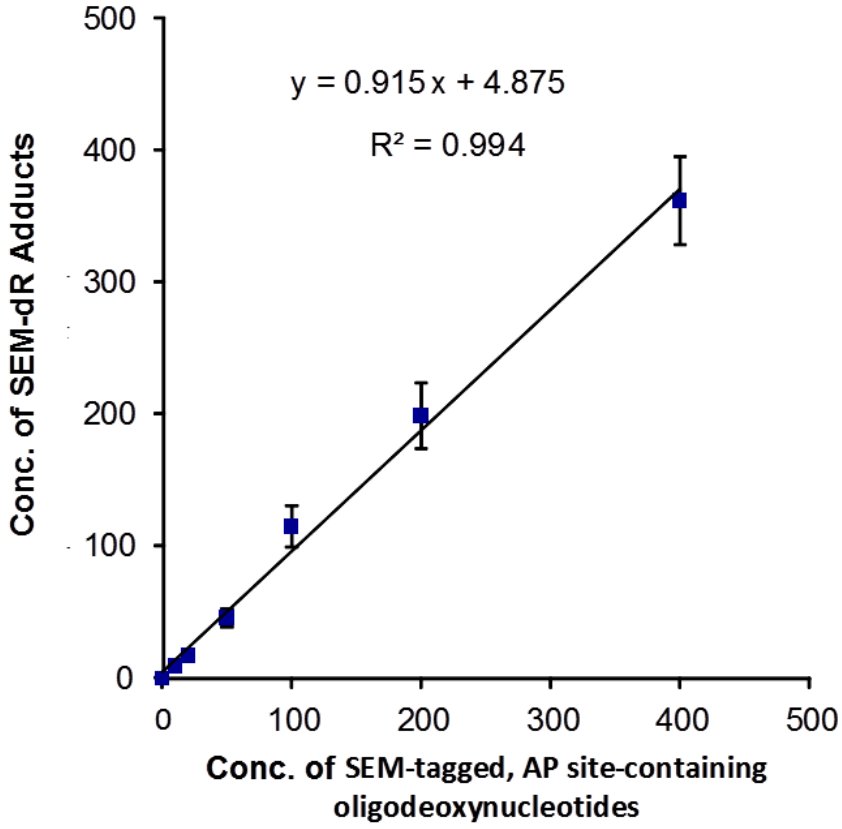

Figure S7 Method validation with synthesized SEM-tagged, AP site-containing oligodeoxynucleotide. The concentration of SEM-dR adduct measured by the developed LC-MS/MS method was directly proportional to the concentration of the oligodeoxynucleotides spiked to the cells. The data represent mean ± SD for three independent experiments