

Supporting Information for

**“6-Thioguanine Perturbs Cytosine Methylation at CpG
Dinucleotide Site by DNA Methyltransferases *in Vitro* and
Acts as a DNA Demethylating Agent *in Vivo*”**

by

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Figure S1. LC-MS/MS for monitoring the restriction fragments of interest with or without methylation at CpG site [i.e. d(pCG^SGTGA) and d(p^mCG^SGTGA), from the BciVI digestion of methylation reaction mixture of Substrate **3**]. Shown in (a) and (b) are the SICs for the formation of indicated fragment ions of the two ODNs, and illustrated in (c) and (d) are the MS/MS of the [M-2H]²⁻ ions of the two ODNs (*m/z* 962.7 and 969.7).

Figure S2. LC-MS/MS for monitoring the restriction fragments of interest with or without methylation at CpG site [i.e. d(TCACCGG) and d(TCAC^mCGG), from the BciVI digestion of the methylation reaction mixture of Substrate **4**]. Depicted in (a) and (b) are the SICs for the formation of indicated fragment ions of these two ODNs, and illustrated in (c) and (d) are the MS/MS of the [M-2H]²⁻ ions of the two ODNs (*m/z* 1039.2 and 1046.2).

Figure S3. HPLC trace for the separation of standard 5-mdC. The HPLC conditions were the same as those described for the separation of nucleoside mixtures from the digestion of genomic DNA isolated from Jurkat cells.

Figure S4. LC-MS/MS analyses of the 5-mdC (a) and guanosine (G, b) fractions. Shown are the extracted-ion chromatograms for the [M + H]⁺ ions of 5-mdC (a) and G (b). Shown in the insets are the MS and MS/MS (for the [M + H]⁺ ions of the two nucleosides). We also monitored the formation of other canonical ribonucleosides and 2'-deoxyribonucleosides; except for the presence of trace amounts of 5-mdC in the G fraction (<2%) and trace amount of G in the 5-mdC fraction (<2%), other nucleosides were not detectable.

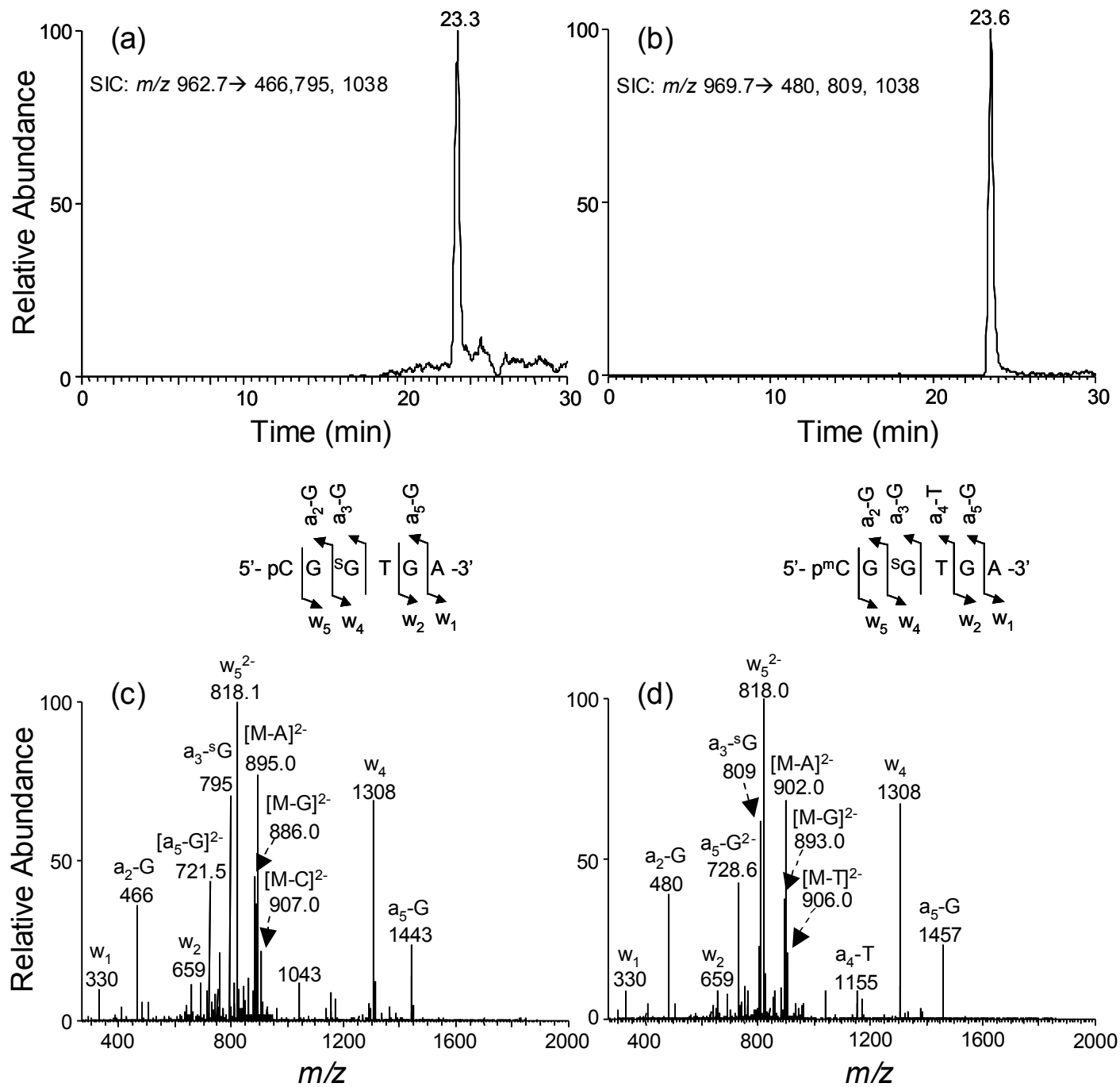


Figure S1

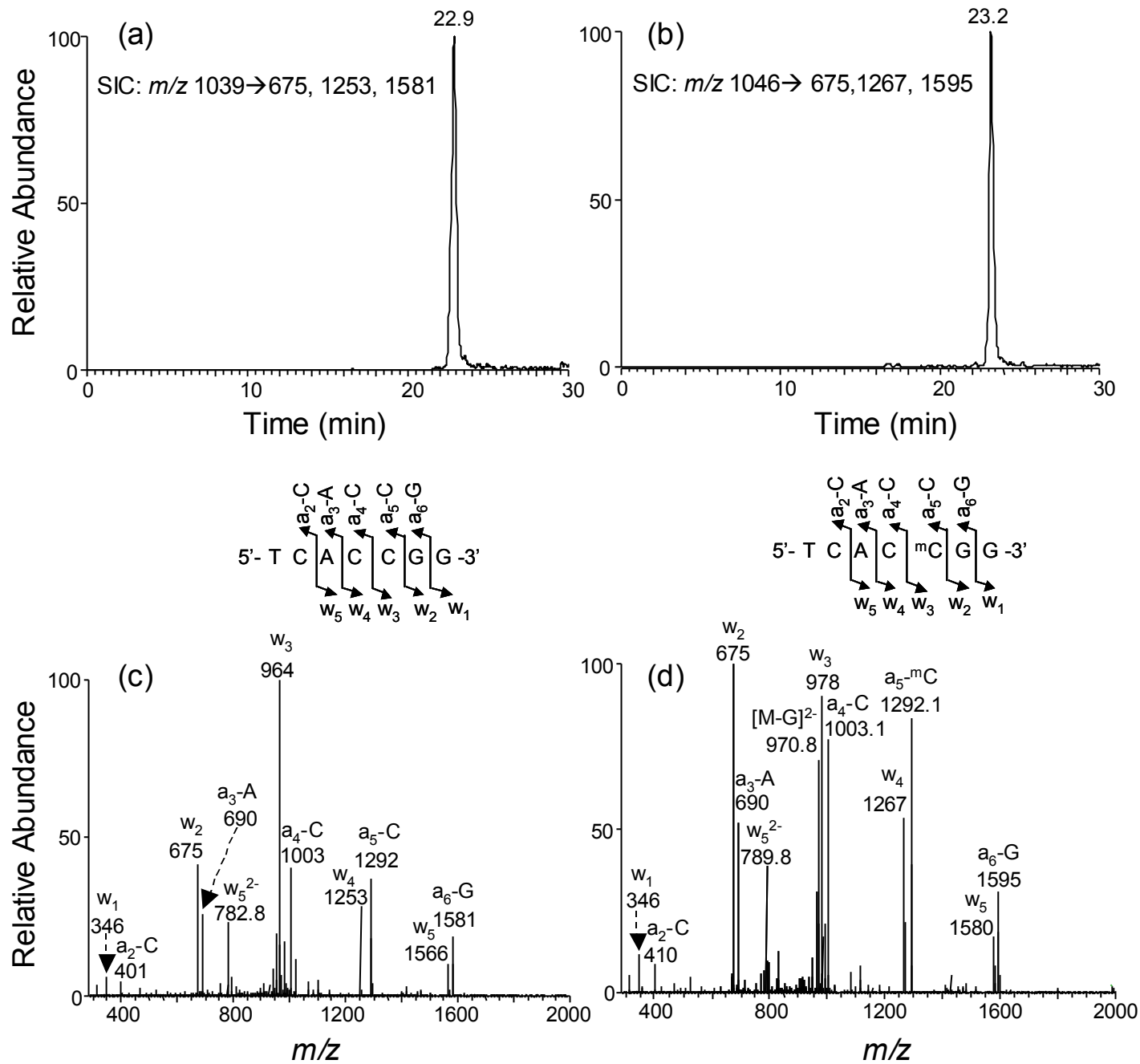


Figure S2

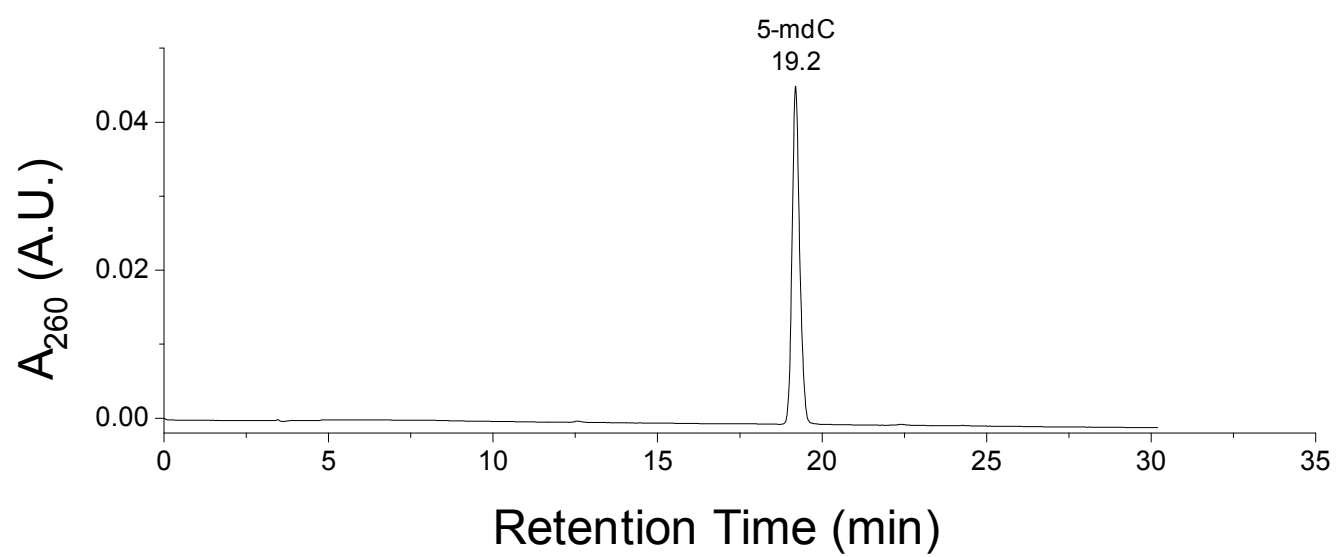


Figure S3

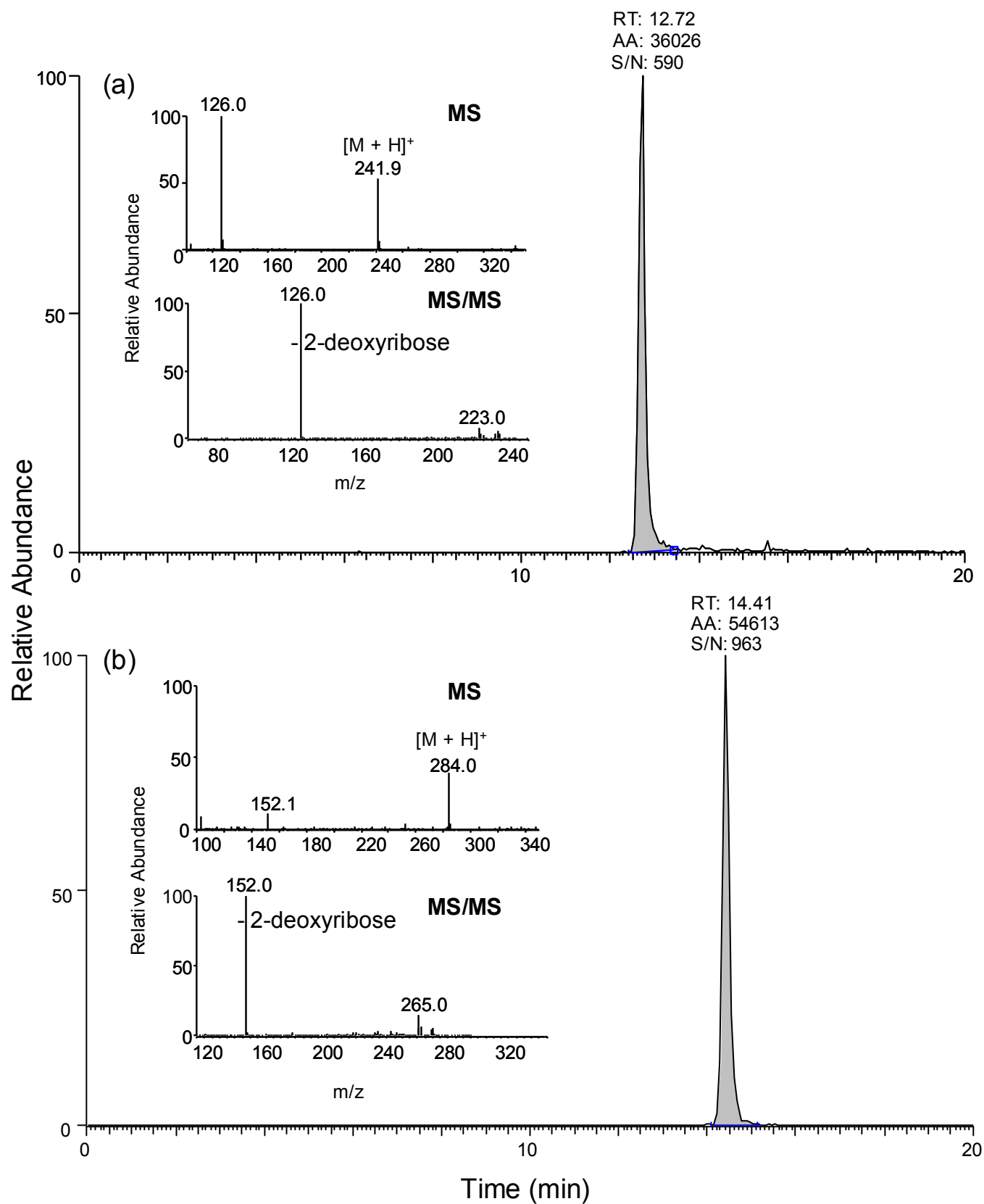


Figure S4