Supporting Information

Analysis of a Malondialdehyde-Deoxyguanosine Adduct in Human Leukocyte DNA by Liquid Chromatography Nanoelectrospray-High Resolution Tandem Mass Spectrometry

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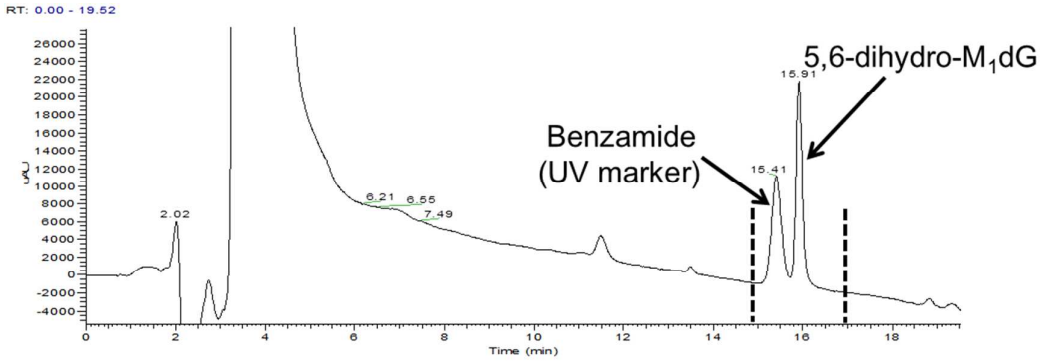

Figure S1. Chromatogram of a standard mixture of benzamide and 5,6-dihydro-M_1dG during column chromatography purification, which was used to further purify human leukocyte DNA samples after SPE extraction. Benzamide was used as a UV marker, and fraction containing 5,6-dihydro-M_1dG and its internal standard at 15~17 min was collected.

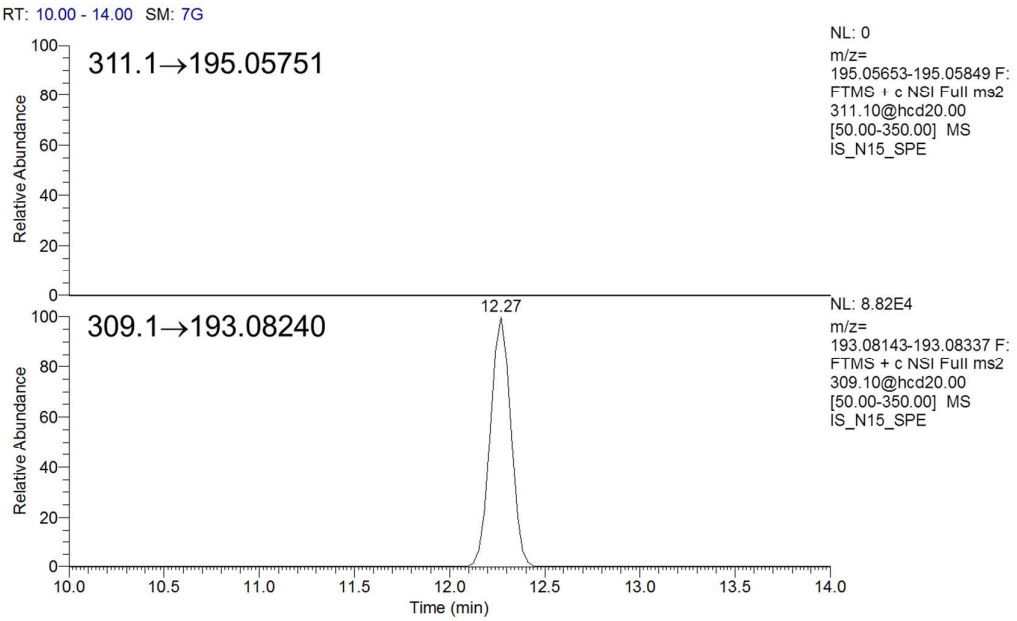

Figure S2. Chromatograms obtained upon analysis of possible artifactual M_1dG production during sample preparation. The internal standards 5,6 dihydro-[$^{13}C_3$]M_1dG and 5,6 dihydro-[$^{15}N_5$]M_1dG are monitored by the MS transition *m/z* 309.1→193.0824 and *m/z* 311.1→195.0575, respectively. No peak of 5,6 dihydro-[$^{15}N_5$]M_1dG was detected, indicating no artifactual M_1dG adduct was formed during the sample preparation.

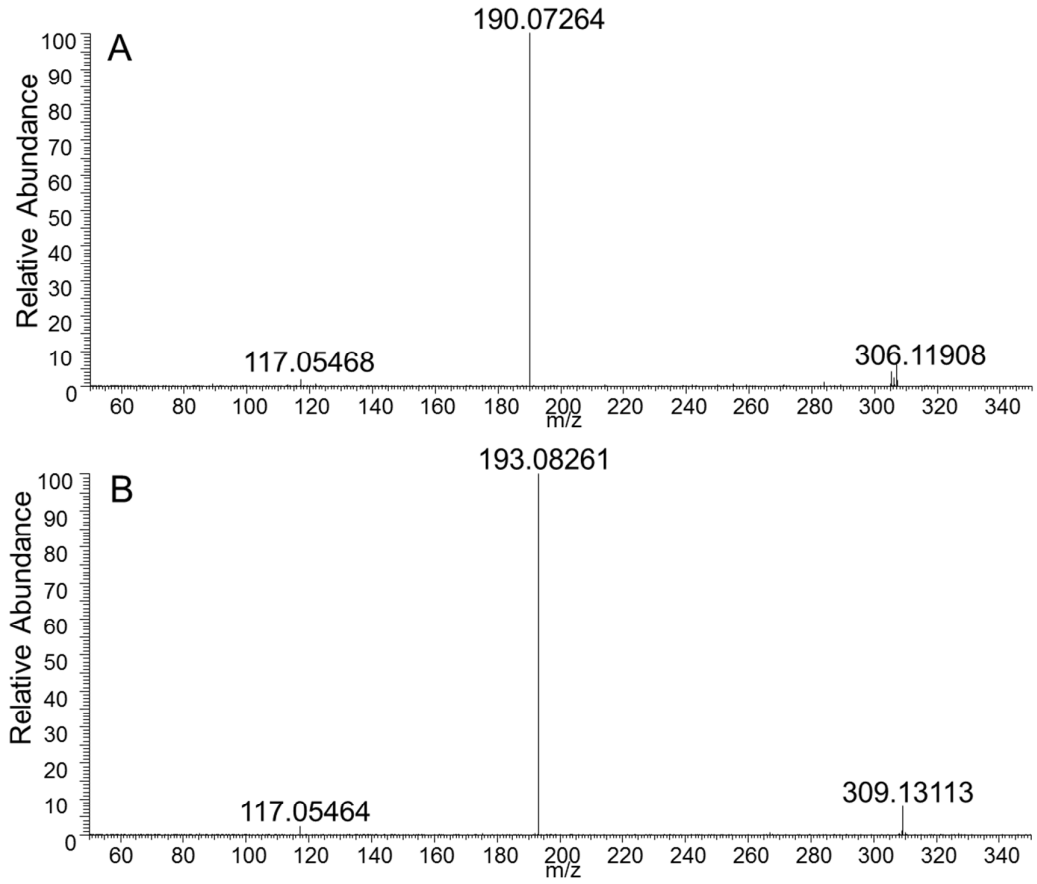

Figure S3. Product ion spectra of (A) 5,6-dihydro-M_1dG, and (B) 5,6-dihydro-[$^{13}C_3$]M_1dG.

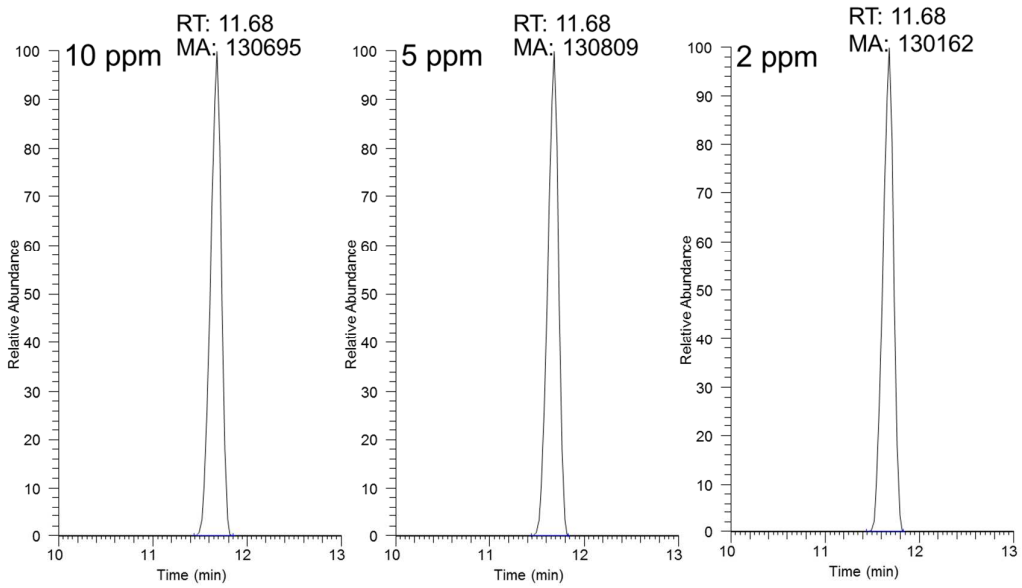

Figure S4. The extracted ion chromatograms for 5,6-dihydro-M_1dG at mass tolerances of (A) 10 ppm, (B) 5 ppm, and (C) 2 ppm using the Orbitrap detector. The MS transition for 5,6-dihydro-M_1dG was *m/z* 306.1→190.0723. No obvious difference was observed when the mass tolerance was set at different values.