

Supporting Information for:

Advanced Glycation End Products of DNA: Quantitative ESI-MS/MS determination of N^2 -(1-carboxyethyl)-2'-deoxyguanosine (CEdG) in biological samples

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Figure S1: UV spectra of stock solutions of unlabeled and isotopically labeled CEdG diastereomers.

Figure S2: ¹H NMR of CEdG(A).

Figure S3: ¹H NMR of CEdG(B).

Figure S4: ¹³C NMR of CEdG(A).

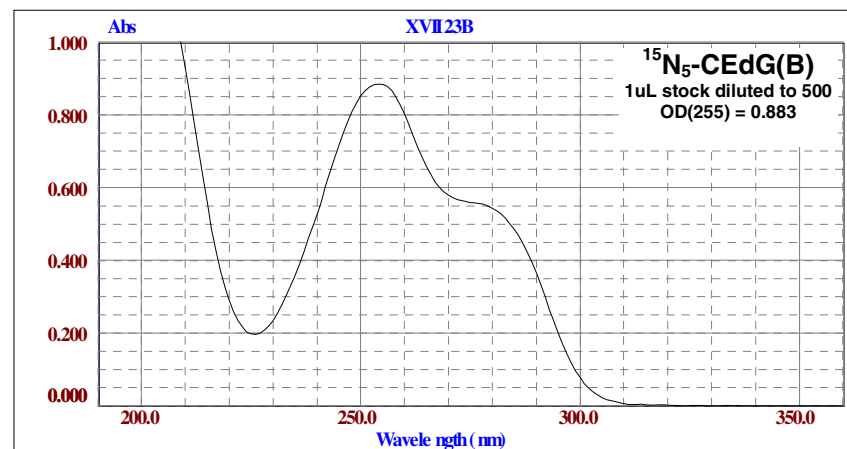
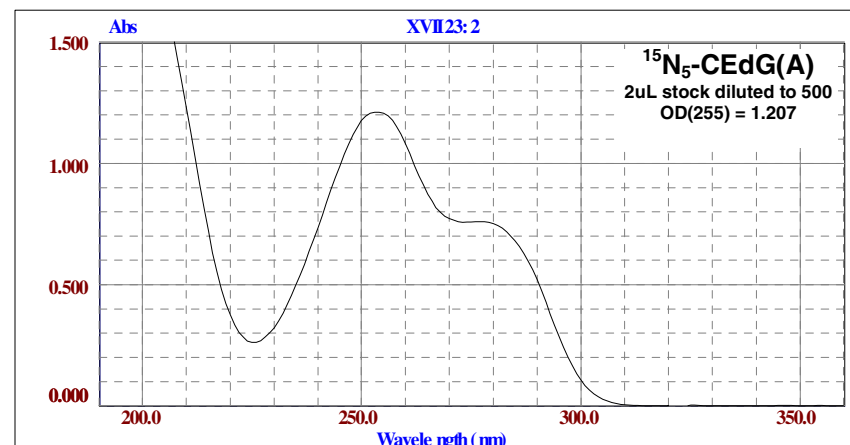
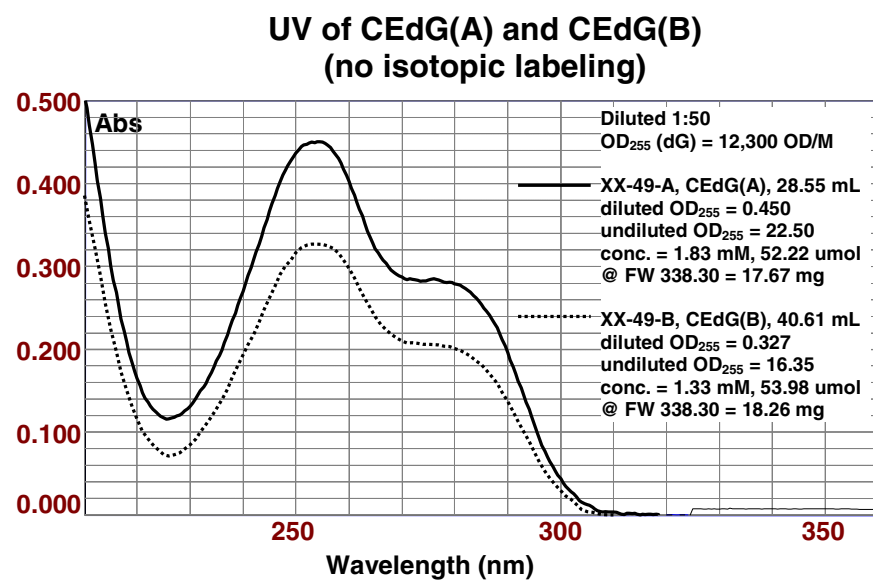
Figure S5: ¹³C NMR of CEdG(B), “b” indicates signals arising from buffer (TEAA).

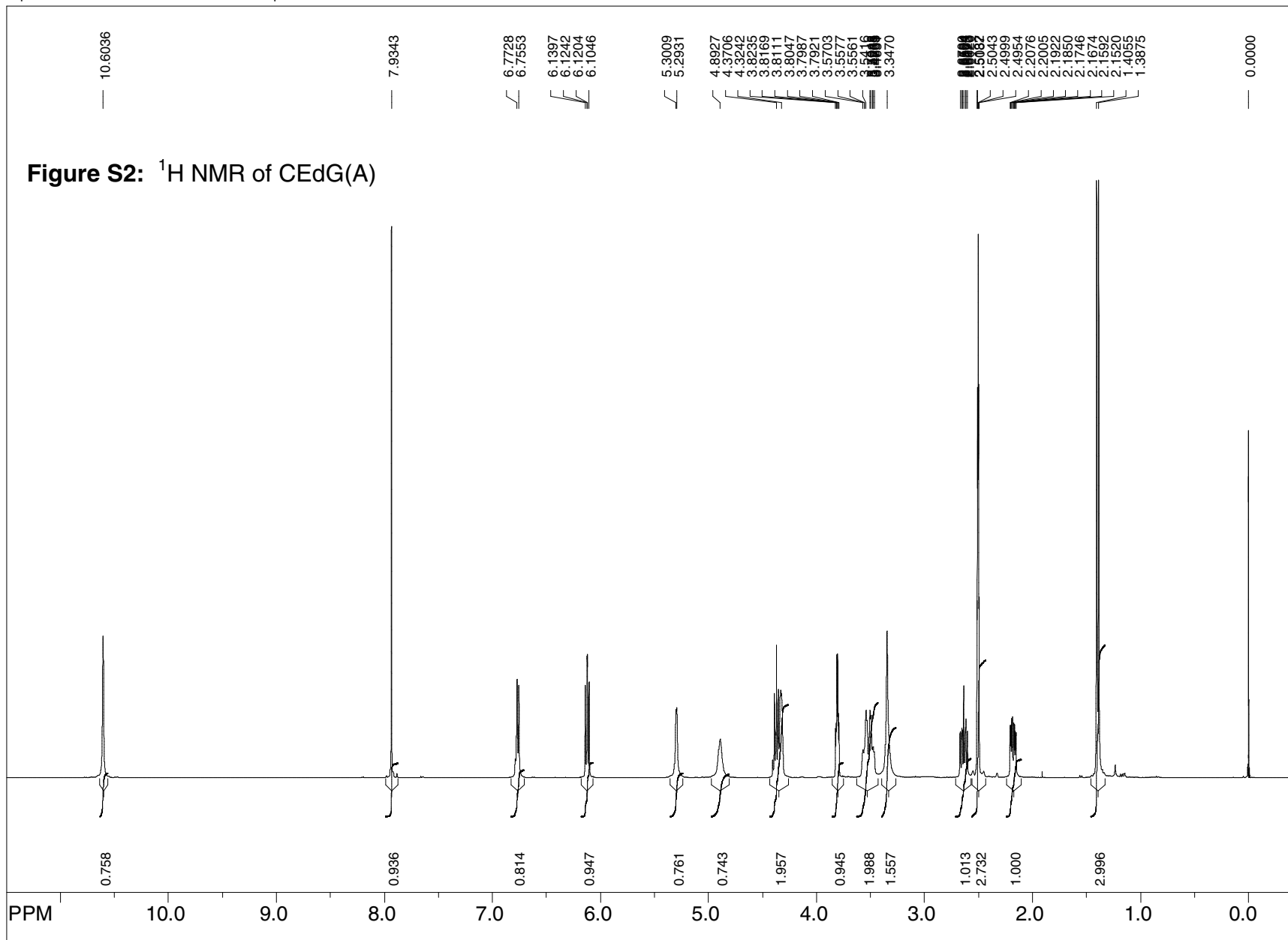
Figure S6: MS2 and MS3 of sodiated CEdG(A) parent ion obtained using the Thermo Finnigan LTQ-FT linear ion trap mass spectrometer.

Figure S7: Product ion scans for CEdG (A) and ¹⁵N₅-CEdG(A) at m/z 340 and 345, respectively, showing the daughter ions at m/z 224 and 229 monitored using a Micromass Quattro Ultima Triple Quadrupole Mass Spectrometer.

Figure S8: Observed isotopic distributions for ¹⁵N₅-CEdG(A) and ¹⁵N₅-CEdG(B) and the calculated isotopic distribution for C₁₃H₁₇¹⁵N₅NaO₆. The latter was calculated using the Molecular Weight Calculator, V. 6.38, by Matthew Monroe, distributed as freeware at <http://www.alchemistmatt.com/>.

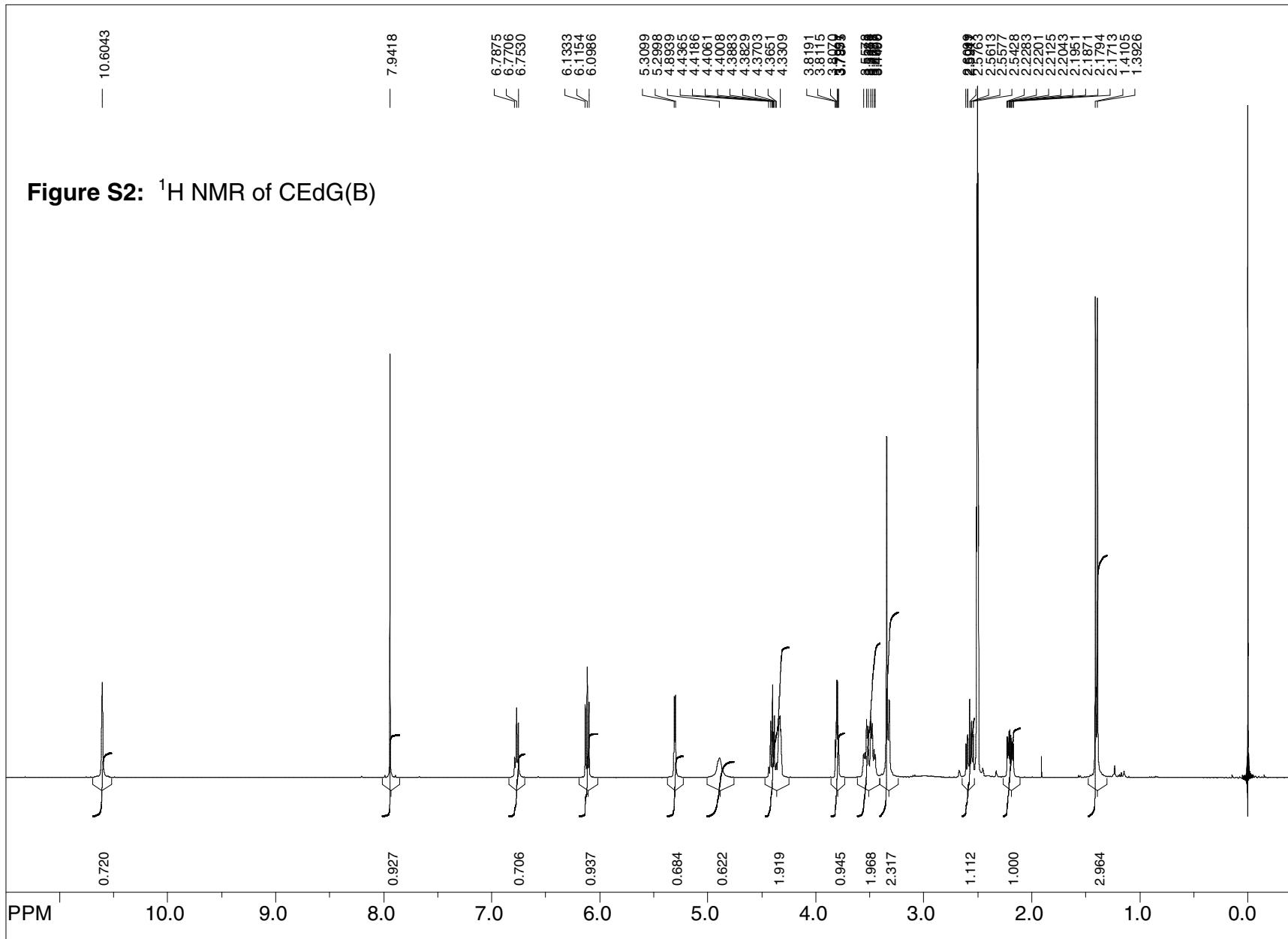
Figure S1: UV spectra of stock solutions of unlabeled and isotopically labeled CEdG diastereomers.





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freq. of 0 ppm: 399.804642 MHz
 processed size: 65536 complex points
 LB: 0.000 GB: 0.0000



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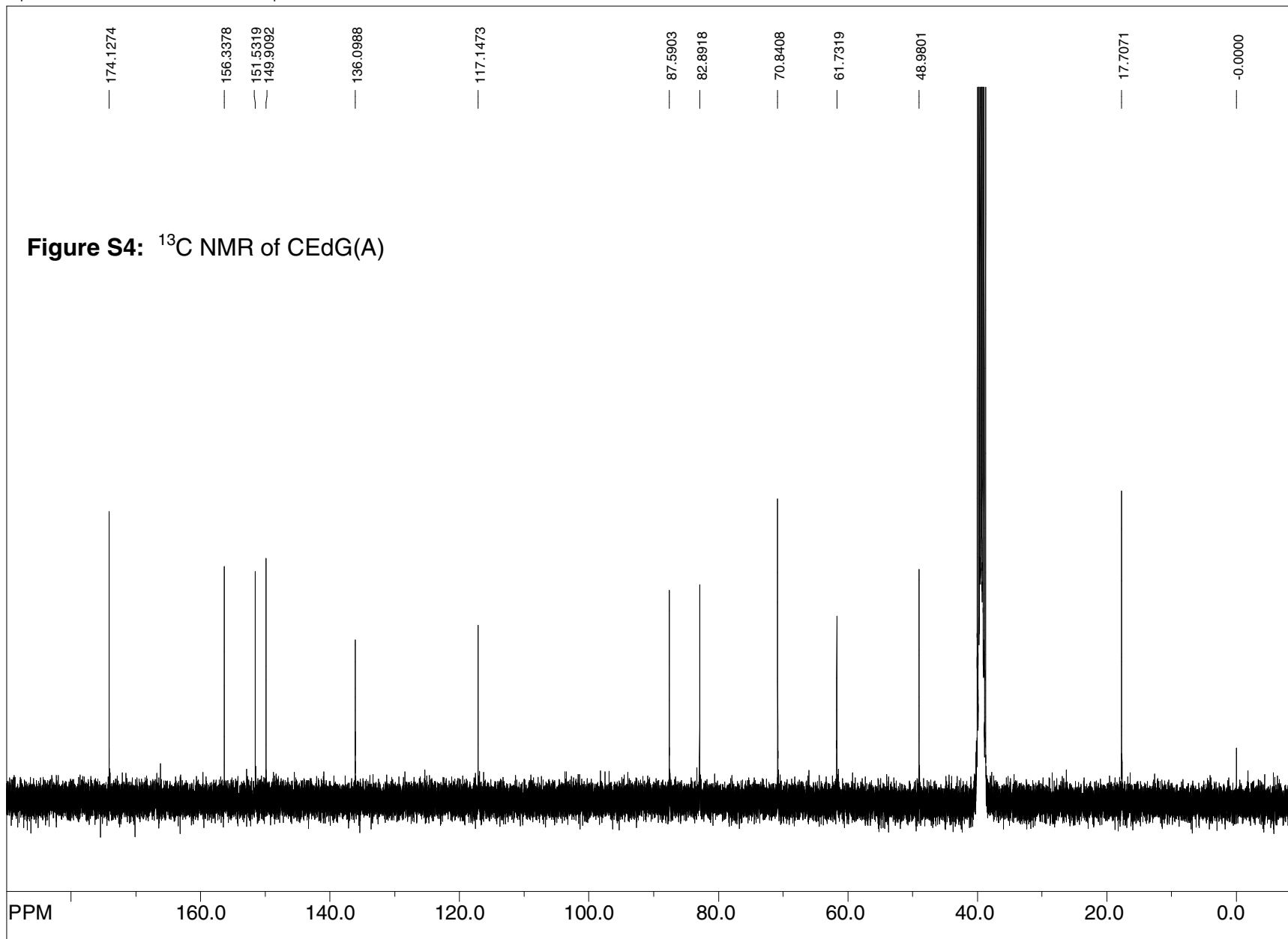


Figure S4: ^{13}C NMR of CE dG(A)

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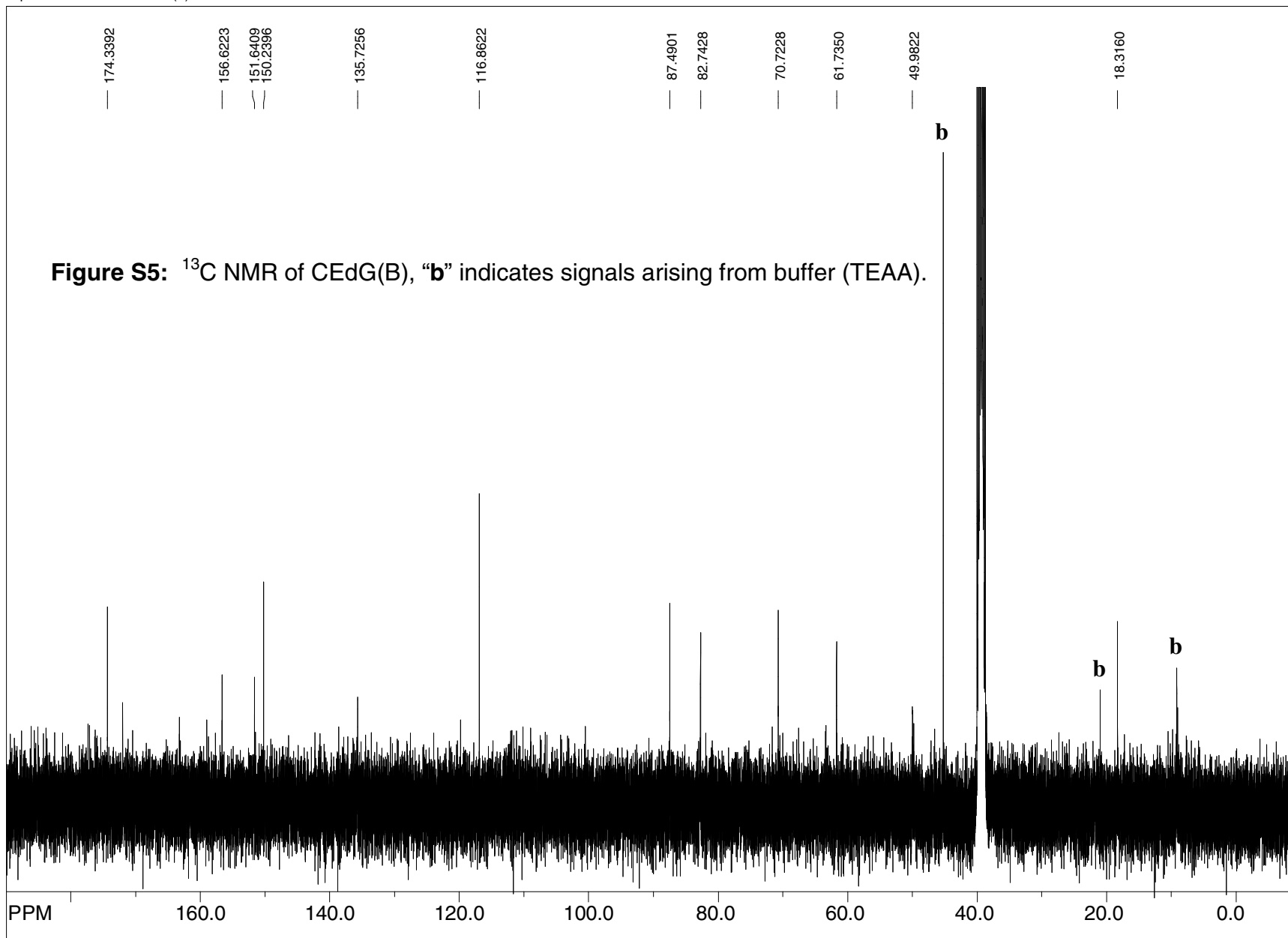


Figure S5: ^{13}C NMR of CEEdG(B), "b" indicates signals arising from buffer (TEAA).

Figure S6: MS2 and MS3 of sodiated CE_dG(A) parent ion obtained using the Thermo Finnigan LTQ-FT linear ion trap mass spectrometer.

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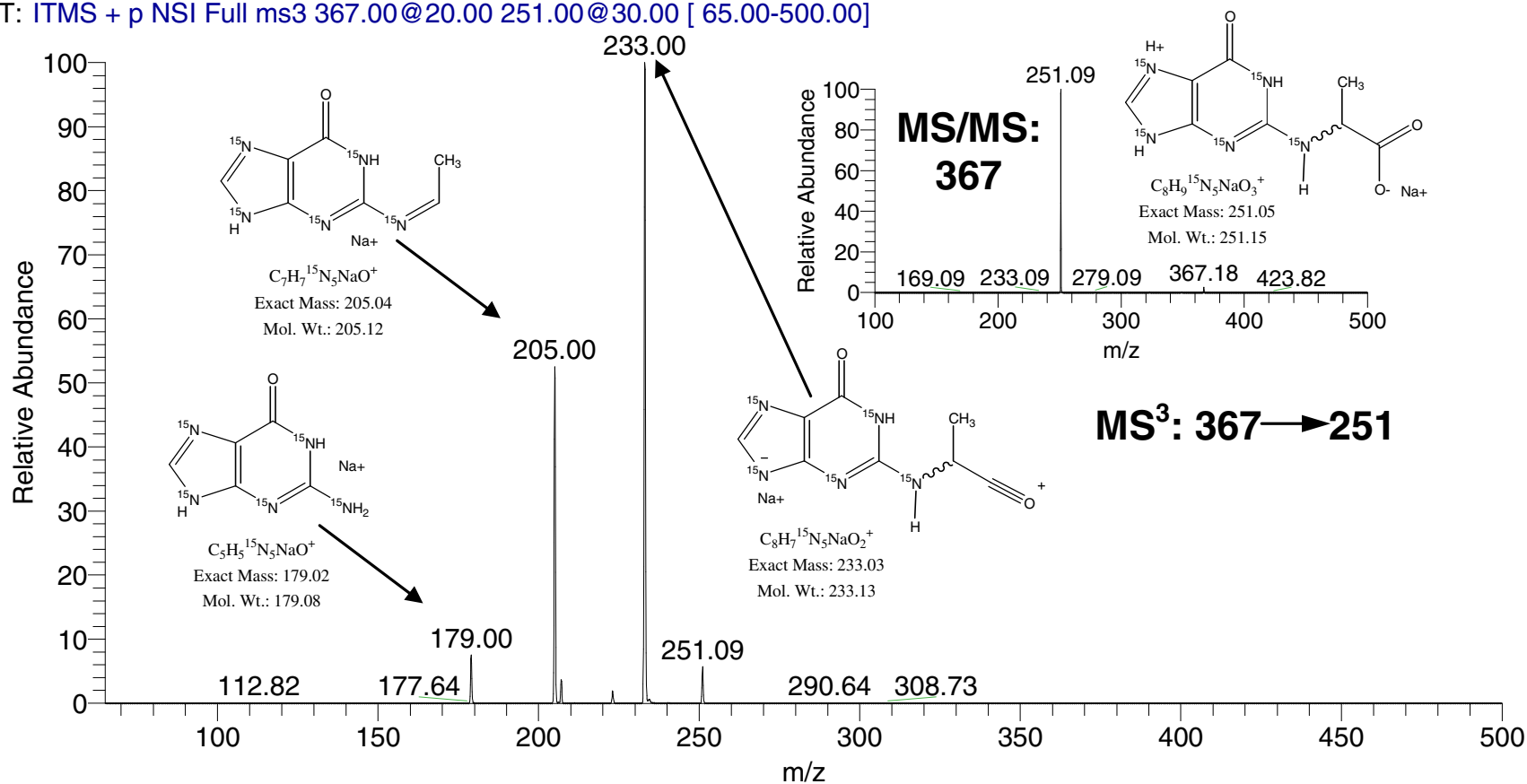


Figure S7. Product ion scans for CEdG (A) and $^{15}\text{N}_5$ -CEdG(A) at m/z 340 and 345, respectively, showing the daughter ions at m/z 224 and 229 monitored using a Micromass Quattro Ultima Triple Quadrupole Mass Spectrometer.

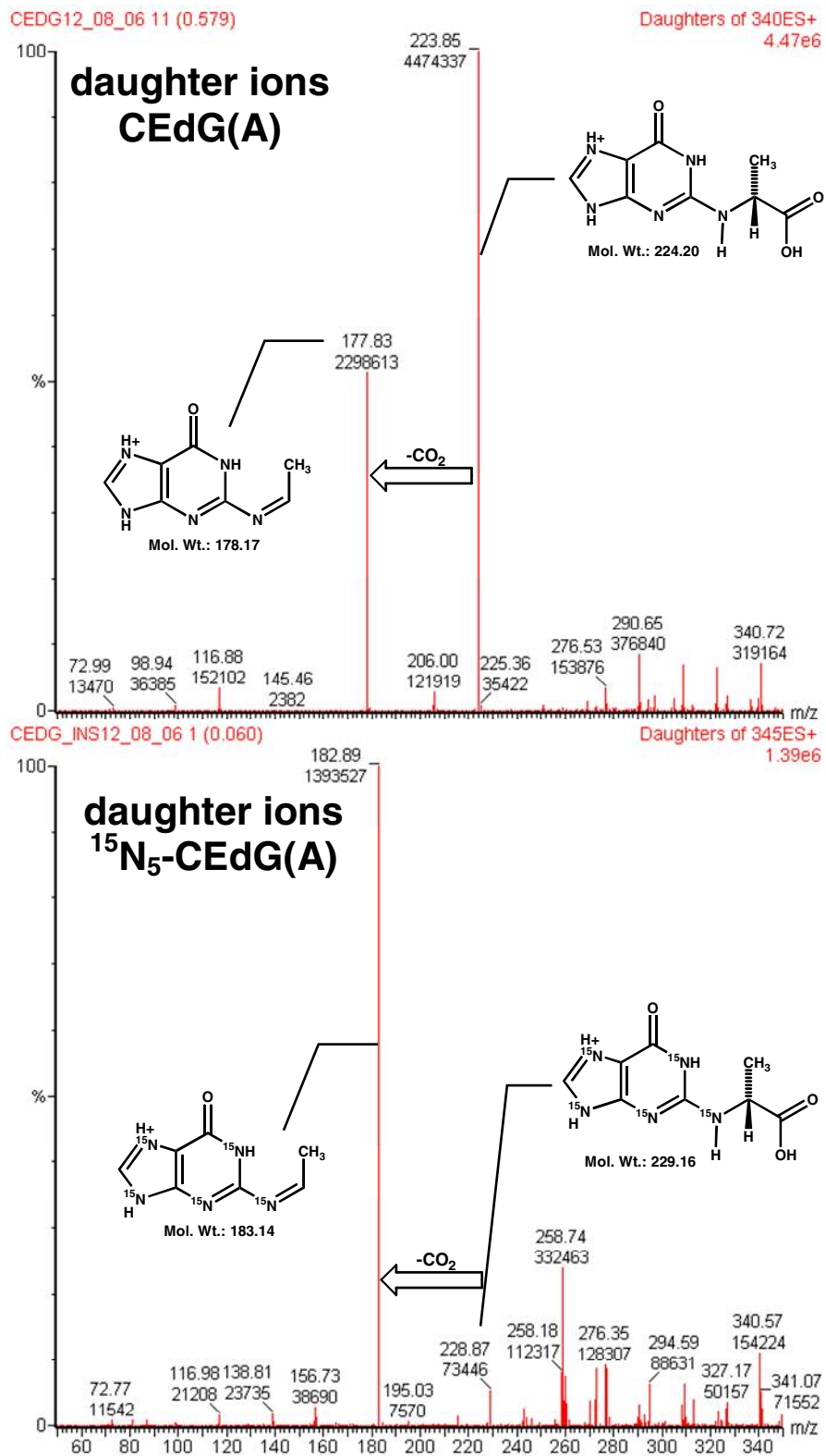
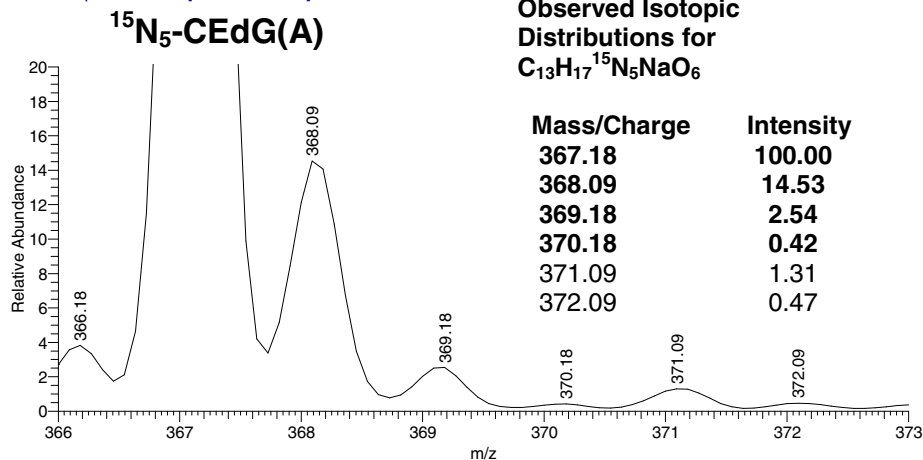


Figure S8: Observed isotopic distributions for $^{15}\text{N}_5\text{-CEdG(A)}$ and $^{15}\text{N}_5\text{-CEdG(B)}$ and the calculated isotopic distribution for $\text{C}_{13}\text{H}_{17}^{15}\text{N}_5\text{NaO}_6$. The latter was calculated using the Molecular Weight Calculator, V. 6.38, by Matthew Monroe, distributed as freeware at <http://www.alchemistmatt.com/>.

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