**Supplemental Information**

**A High Resolution/Accurate Mass (HRAM) Data-Dependent MS3 Neutral Loss Screening, Classification, and Relative Quantitation Methodology for Carbonyl Compounds in Saliva**

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Submitted to *Journal of the American Society for Mass Spectrometry* for consideration as a *Research Article*

**Supporting Tables**

**Supporting Table 1.** Limits of detection on column (LOD) of DNPH-derivatized carbonyls in water.



\*LOD on column

**Supporting Table 2.** Limits of detection on column (LOD) of DNPH-derivatized carbonyls in saliva as matrix.



\*LOD on column

**Supporting Figures**



**Supporting Figure 1.** Experimental scheme for characterizing carbonyl exposures.



**Supporting Figure 2.** MS2 and MS3 fragmentation of DNPH-derivatized aliphatic/saturated aldehydes using nano-ESI in positive ionization mode.



**Supporting Figure 2 (cont.).** MS2 and MS3 fragmentation of DNPH-derivatized aliphatic/saturated aldehydes using nano-ESI in positive ionization mode.



**Supporting Figure 3.** MS2 and MS3 fragmentation of DNPH-derivatized aldehydes containing aromatic groups using nano-ESI in positive ionization mode.



**Supporting Figure 3 (cont.).** MS2 and MS3 fragmentation of DNPH-derivatized aldehydes containing aromatic groups using nano-ESI in positive ionization mode.



**Supporting Figure 4.** MS2 and MS3 fragmentation of DNPH-derivatized aliphatic/unsaturated aldehydes using nano-ESI in positive ionization mode.



**Supporting Figure 5.** MS2 and MS3 fragmentation of DNPH-derivatized aliphatic ketones using nano-ESI in positive ionization mode.



**Supporting Figure 6.** MS2 and MS3 fragmentation of DNPH-derivatized ketones containing cyclic/aromatic groups using nano-ESI in positive ionization mode.



**Supporting Figure 7.** MS2 and MS3 fragmentation of DNPH-derivatized dicarbonyls using nano-ESI in positive ionization mode.



**Supporting Figure 8.** Proposed fragmentation pathways and structures of the neutral losses and characteristic ions used for structural elucidation of DNPH-derivatized carbonyls containing aromatic groups.



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**Supporting Figure 9.** Fragmentation pathways and proposed structures of the neutral losses and characteristic ions used for structural elucidation of DNPH-derivatized aliphatic carbonyls.