Supplemental Information for: Optimization of Confined Direct Analysis in Real Time Mass Spectrometry (DART-MS)

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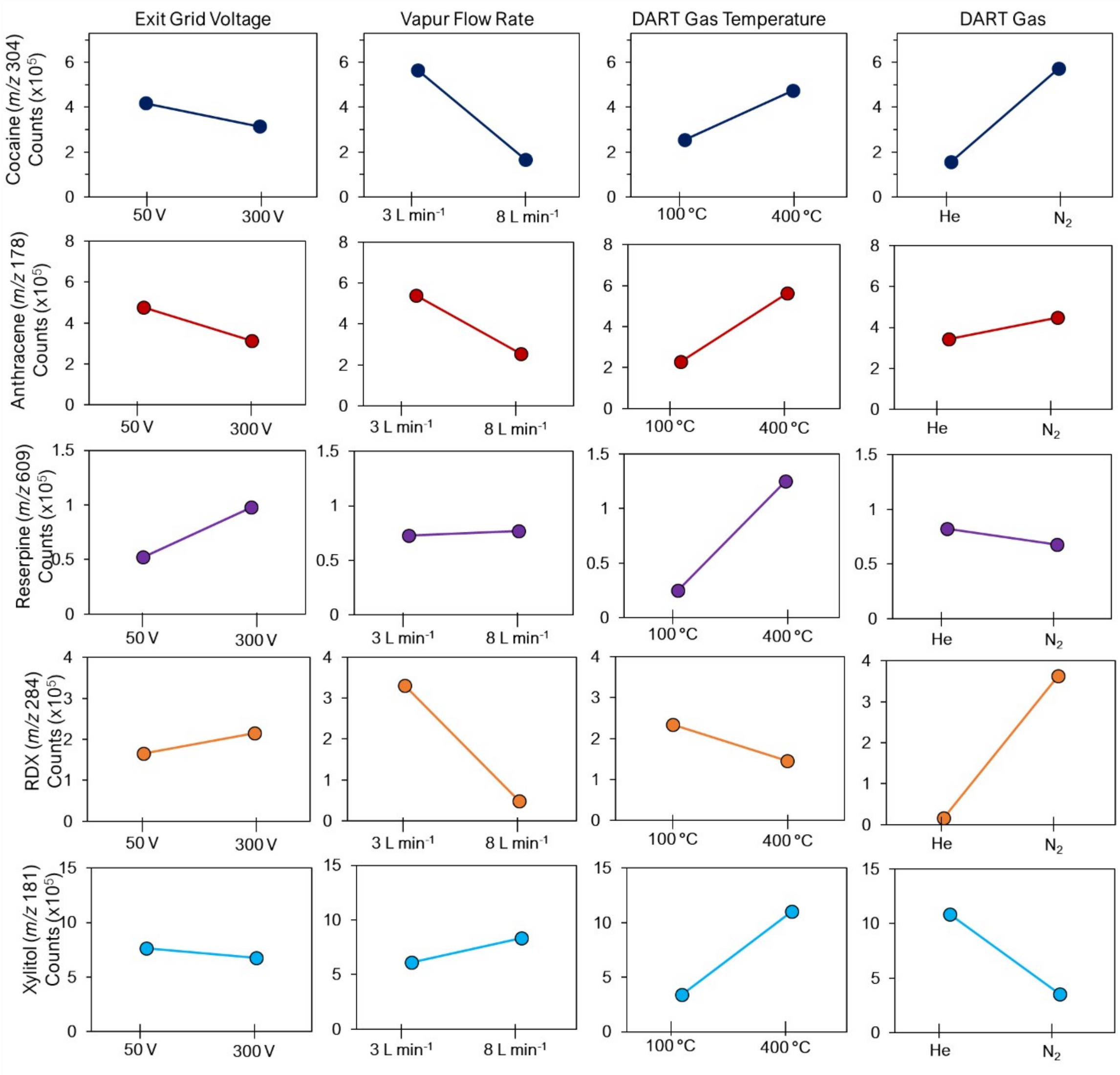

Figure S1. Main effects plots from the partial factorial design of experiments study for cocaine (navy blue), anthracene (red), reserpine (purple), RDX (orange), and xylitol (light blue).

Table S1. Parameters and results for each setting of the design of experiments study.

Run #	1	2	3	4
DART Exit Grid (V)	50	300	50	300
Vapur Flow (L min^{-1})	3	3	8	8
DART Gas Temp (°C)	100	100	100	100
DART Gas	He	N_2	N_2	He
Average Analyte Response (counts)				
Anthracene	15317	22315	23781	29661
Cocaine	109676	558434	238130	114943
Reserpine	17048	14829	41560	25995
RDX	38215	776070	111807	11353
Xylitol	280587	103244	297411	675226
Run #	**5**	**6**	**7**	**8**
DART Exit Grid (V)	50	300	50	300
Vapur Flow (L min^{-1})	3	3	8	8
DART Gas Temp (°C)	400	400	400	400
DART Gas	N_2	He	He	N_2
Average Analyte Response (counts)				
Anthracene	118735	58926	33074	14749
Cocaine	1251219	337861	66962	242630
Reserpine	61947	197617	87768	152391
RDX	502752	6604	6909	64468
Xylitol	576177	1476943	1911240	445836

Table S2. Valve dial positions for select Vapur flow rates used in this study.

Vapur Flow Rate (L min^{-1})	2	3	4	5	6	7	8
Dial Position	2.5	3.5	5.0	7.0	8.5	0.0	1.0
	1st Turn (Red Band)					2nd Turn (Blue Band)	

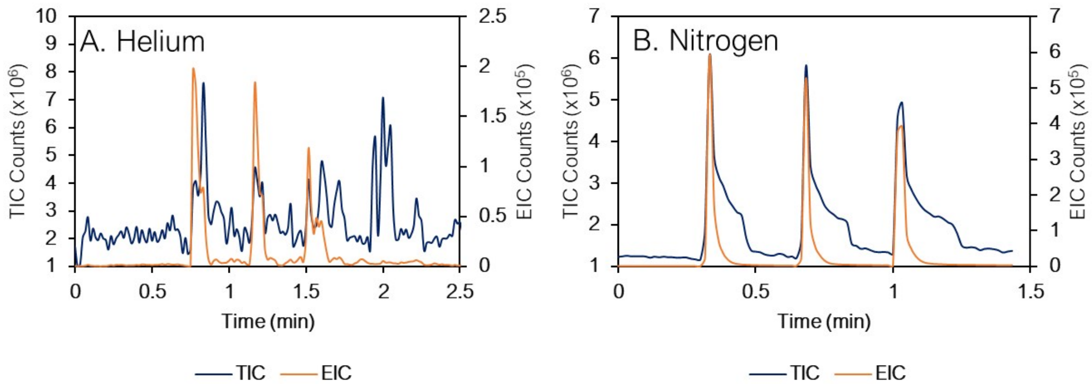

Figure S2. Example total ion chronographs (TICs, blue trace) and corresponding extracted ion chronographs (EICs, orange trace) of cocaine when using (A.) helium and (B.) nitrogen at a Vapur flow rate of 4.5 L min^{-1}.

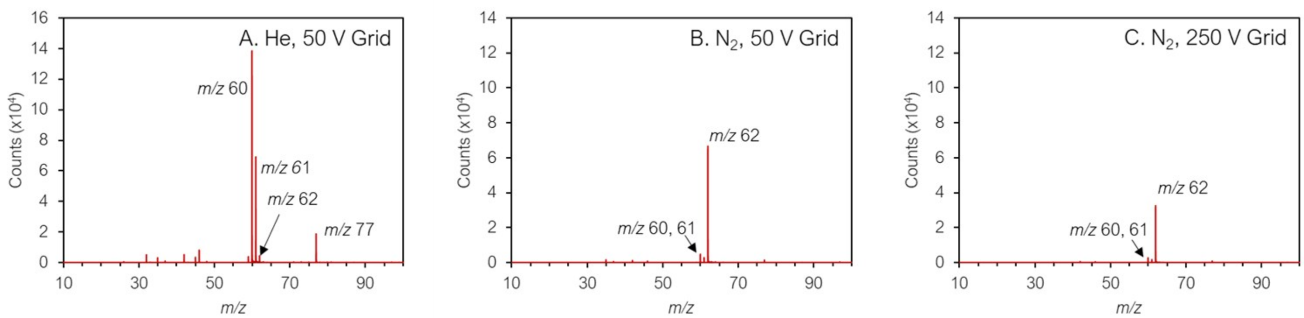

Figure S3. Negative mode background spectra when using helium (A.) and nitrogen (B. and C.) as the DART ionization gas. Also shown is background spectra using a -50 V DART exit grid voltage (B.) and a voltage of -250 V.

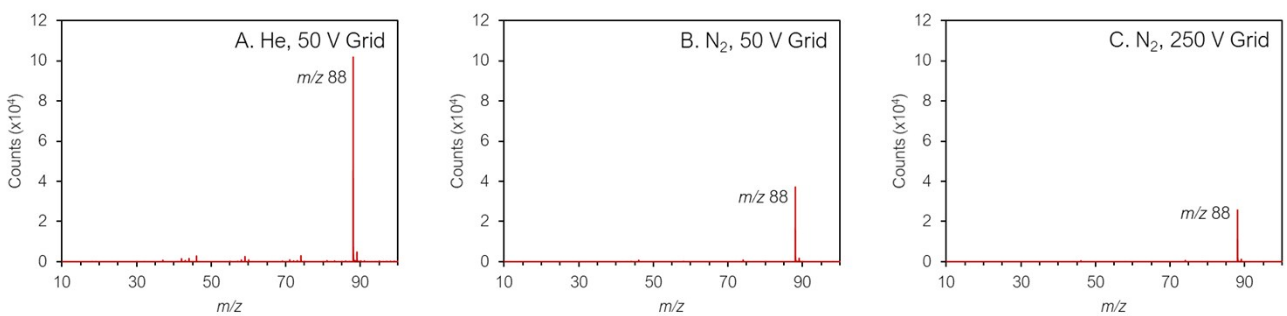

Figure S4 Positive mode background spectra when using helium (A.) and nitrogen (B. and C.) as the DART ionization gas. Also shown is background spectra using a +50 V DART exit grid voltage (B.) and a voltage of +250 V.

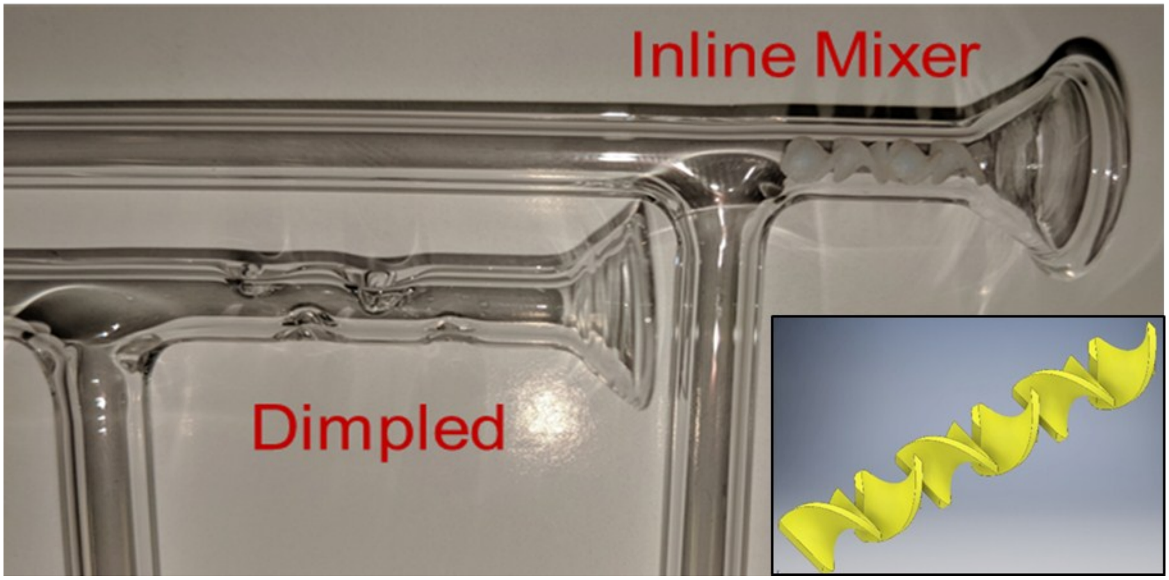

Figure S5. Photo of inline mixer (top) and dimpled junction (bottom) modifications. A CAD drawing of the inline mixer is shown in the inset of the figure.

Supplemental Videos

Video S1. Schlieren imaging of the TD-DART front end at increasing Vapur flow rates when using nitrogen as the DART ionization gas.

Video S2. Schlieren imaging of the TD-DART front end at increasing Vapur flow rates when using helium as the DART ionization gas.

Video S3. High-speed video of the TD-DART junction when using helium and nitrogen at a Vapur flow rate of 3.5 L min^{-1}. Theatrical fog was used to simulate the analyte vapor.

Video S4. High-speed video of the TD-DART junction when using helium and nitrogen at a Vapur flow rate of 8 L min^{-1}. Theatrical fog was used to simulate the analyte vapor.

Video S5. High-speed video of the TD-DART junction containing the in-line mixer modification using helium and a Vapur flow rate of 3.5 L min^{-1}. Theatrical fog was used to simulate the analyte vapor.

Video S6. High-speed video of the TD-DART junction with the dimple modification when using helium and nitrogen at a Vapur flow rate of 3.5 L min^{-1}. Theatrical fog was used to simulate the analyte vapor.

Video S7. Schlieren imaging of the TD-DART front end, using the dimple modification, at increasing Vapur flow rates when using helium as the DART ionization gas.