# **Supporting Information for:** Method for Evaluating Ion Mobility Spectrometers for Trace Detection of Fentanyl and Fentanyl-related Substances

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**Table S1.** Measured K<sub>0</sub> (K<sub>0</sub><sup>meas</sup>) for fentanyl and fentanyl-related compounds for individual instruments used in main work. Additional K<sub>0</sub><sup>meas</sup> for single instruments from cited references [1-3]. Calculated K<sub>0</sub> (K<sub>0</sub><sup>calc</sup>) from polynomial equation described in main work. Compounds sorted according to those reported in Table 1 of main work, followed by additional fentanyl-related compounds found in an internet search and sorted by molecular weight. Additional fentanyl-related substances drawn primarily from Traceable Opioid Material Kits to Improve Laboratory Detection of Synthetic Opioids in the U.S. provided by the Centers for Disease Control and Prevention (CDC) at https://www.cdc.gov/nceh/dls/erb\_opioid\_kits.html.

Compo	und		te calc					$K_0^{meas}$	cm <sup>2</sup> V <sup>-1</sup>	s⁻¹)			
Name	Formula	MW	(cm <sup>2</sup> V <sup>-1</sup> s <sup>-1</sup> )		Indi	vidual P	latforms	s, this st	udy		[1]	[2]	[3]
		(Da)		1	2	3	4	5	6	7			
Fentanyl	$C_{22}H_{28}N_2O$	336.47	1.057	1.052	1.052	1.058	1.056	1.059	1.052	1.065	1.050	1.049	1.049
Furanyl fentanyl	$C_{24}H_{26}N_2O_2$	374.47	0.999	1.003	1.003	1.012	1.006	1.011	1.005	1.021	1.000	1.000	1.000
Acetyl fentanyl	$C_{21}H_{26}N_2O$	322.44	1.083	1.081	1.083	1.088	1.081	1.089	1.085	1.094	1.080	1.080	1.079
FIBF	$C_{23}H_{29}FN_2O$	368.49	1.007	1.006	1.002	1.013	1.006	1.012	1.006	1.022	1.000	1.002	1.002
Carfentanil	$C_{24}H_{30}N_2O_3$	394.51	0.975	0.976	0.976	0.980	0.981	0.984	0.976	0.990	0.970	0.971	0.971
4-ANPP	$C_{19}H_{24}N_2$	280.41	1.175	1.170	1.173	1.182	1.179	1.171	1.160				1.172
Butyryl fentanyl	$C_{23}H_{30}N_2O$	350.50	1.034	1.022	1.021	1.030	1.025	1.030	1.023	1.036	1.020	1.018	1.018
Acrylfentanyl	$C_{22}H_{26}N_2O$	334.45	1.061	1.061	1.061	1.066	1.065	1.069	1.063	1.073		1.057	1.057
(±)- <i>trans</i> -3-methyl Fentanyl	$C_{23}H_{30}N_2O$	350.50	1.034	1.026	1.020	1.034	1.024	1.027	1.025	1.037		1.022	
U-47700	$C_{16}H_{22}CI_2N_2O$	329.26	1.070	1.091	1.092	1.096	1.096	1.099	1.090	1.094		1.091	1.091

Cyclopropyl fentanyl	$C_{23}H_{28}N_2O$	348.48	1.037	1.029	1.031	1.036	1.034	1.033	1.030	1.044			
Methoxyacetyl fentanyl	$C_{22}H_{28}N_2O_2$	352.47	1.031										1.031
Valeryl fentanyl	$C_{24}H_{32}N_2O$	364.52	1.013	0.990	0.989	0.999	0.993	0.997	0.991	1.008		0.987	0.986
<i>ortho</i> -Fluorobutyryl fentanyl	$C_{23}H_{29}FN_2O$	368.49	1.007									1.011	
ortho-Fluorofentanyl	C <sub>22</sub> H <sub>27</sub> FN <sub>2</sub> O	354.46	1.027										1.040
Thiophene fentanyl	$C_{24}H_{26}N_2OS$	390.54	0.980										
Benzyl fentanyl	$C_{21}H_{26}N_2O$	322.44	1.083	1.083	1.085	1.088	1.088	1.092	1.081	1.088		1.082	
U-49900	$C_{18}H_{26}CI_2N_2O$	357.32	1.023										
NPP	C <sub>13</sub> H <sub>17</sub> NO	203.28	1.400										
β-Hydroxythiofentanyl	$C_{20}H_{26}N_2O_2S$	358.50	1.021								1.030	1.029	1.026
Acetyl norfentanyl	$C_{13}H_{18}N_2O$	218.29	1.351	1.357	1.363	1.357	1.356	1.362	1.353	1.337			
α-methyl Acetyl fentanyl	C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O	336.47	1.057										
Tetrahydrofuran fentanyl	$C_{24}H_{30}N_2O_2$	378.51	0.994										
U-48800	$C_{17}H_{24}CI_2N_2O$	343.29	1.046										
Benzoylbenzyl fentanyl	$C_{25}H_{26}N_2O$	370.49	1.004										
			End	, Table	e 1 Con	npoune	ds						
Norfentanyl	$C_{14}H_{20}N_2O$	232.32	1.307	1.301	1.305	1.301	1.302	1.308	1.299	1.287			

Butyryl norfentanyl	$C_{16}H_{22}N_2O$	246.35	1.266						
N-methyl Cyclopropyl norfentanyl	$C_{16}H_{22}N_2O$	258.36	1.232						
Furanyl norfentanyl	$C_{16}H_{18}N_2O_2$	270.33	1.201						
Norsufentanil	$C_{16}H_{24}N_2O_2$	276.37	1.185						
Norcarfentanil	$C_{16}H_{22}N_2O_3$	290.36	1.152						
Despropionyl <i>ortho-</i> Methylfentanyl	$C_{20}H_{26}N_2$	294.43	1.142						
Despropionyl fentanyl	$C_{19}H_{23}FN_2$	298.40	1.133				1.170	1.144	
Despropionyl <i>ortho-</i> fluorofentanyl	$C_{19}H_{23}FN_2$	298.40	1.133						
N-methyl Norcarfentanil	$C_{17}H_{24}N_2O_3$	304.38	1.120						
Benzyl Acrylfentanyl	$C_{21}H_{24}N_2O$	320.43	1.087						
Furanylethyl fentanyl	$C_{20}H_{26}N_2O_2$	326.43	1.076						
Thienyl fentanyl	$C_{19}H_{24}N_2O$	328.47	1.072						
AH 7921	$C_{16}H_{22}CI_2N_2O$	329.26	1.070						1.084
4'-methyl Acetyl fentanyl	$C_{22}H_{28}N_2O$	336.47	1.057						
<i>ortho</i> -methyl Acetyl fentanyl	$C_{22}H_{28}N_2O$	336.47	1.057						

β-methyl Acetyl fentanyl	$C_{22}H_{28}N_2O$	336.47	1.057									
<i>para</i> -methyl Acetyl fentanyl	$C_{22}H_{28}N_2O$	336.47	1.057									
Fentanyl Methyl Carbamate	$C_{21}H_{26}N_2O_2$	338.44	1.054									
2,3-seco-Fentanyl	$C_{22}H_{30}N_2O$	338.49	1.054									
<i>para</i> -Fluoroacetyl fentanyl	$C_{21}H_{25}FN_2O$	340.43	1.050									
Thiofentanyl	$C_{20}H_{26}N_2OS$	342.50	1.047									
β- Hydroxythioacetylfentanyl	$C_{19}H_{24}N_2O_2S$	344.47	1.044									
Crotonyl fentanyl	$C_{23}H_{28}N_2O$	348.48	1.037	1.018	1.020	1.026	1.020	1.023	1.025	1.035		
<i>ortho</i> -methyl Acrylfentanyl	$C_{23}H_{28}N_2O$	348.48	1.037									
Methacrylfentanyl	$C_{23}H_{28}N_2O$	348.48	1.037									
para-methyl Acrylfentanyl	$C_{23}H_{28}N_2O$	348.48	1.037									
MT-45	$C_{24}H_{32}N_2$	348.52	1.037									0.998
Isobutyryl fentanyl	$C_{23}H_{30}N_2O$	350.50	1.034								1.020	
(±)- <i>cis</i> -3-methyl Fentanyl	$C_{23}H_{30}N_2O$	350.50	1.034									1.029
meta-Methylfentanyl	$C_{23}H_{30}N_2O$	350.50	1.034									

4'-methyl Fentanyl	$C_{23}H_{30}N_2O$	350.50	1.034					
ortho-Methylfentanyl	$C_{23}H_{30}N_2O$	350.50	1.034					
para-Methylfentanyl	$C_{23}H_{30}N_2O$	350.50	1.034					
β-methyl Fentanyl	$C_{23}H_{30}N_2O$	350.50	1.034					
α-methyl Fentanyl	$C_{23}H_{30}N_2O$	350.50	1.034					
N,N-Dimethylamido- despropionyl fentanyl	$C_{22}H_{29}N_3O$	351.48	1.032					
ortho-fluoro Acrylfentanyl	$C_{22}H_{25}FN_2O$	352.44	1.031					
para-fluoro Acrylfentanyl	$C_{22}H_{25}FN_2O$	352.44	1.031					
Fentanyl Carbamate	$C_{22}H_{28}N_2O_2$	352.47	1.031					
<i>para</i> -methoxy Acetyl fentanyl	$C_{22}H_{28}N_2O_2$	352.47	1.031					
β-hydroxy Fentanyl	$C_{22}H_{28}N_2O_2$	352.47	1.031					
<i>meta</i> -Fluorofentanyl	$C_{22}H_{27}FN_2O$	354.46	1.027					
<i>para</i> -Fluorofentanyl	$C_{22}H_{27}FN_2O$	354.46	1.027					1.030
4'-Fluorofentanyl	$C_{22}H_{27}FN_2O$	354.46	1.027					
α-methyl Thiofentanyl	$C_{21}H_{28}N_2OS$	356.52	1.024					
(±)- <i>trans</i> -3-methyl Thiofentanyl	$C_{21}H_{28}N_2OS$	356.52	1.024					

(±)- <i>cis</i> -3-methyl Thiofentanyl	$C_{21}H_{28}N_2OS$	356.52	1.024					
Isopropyl U-47700	$C_{18}H_{26}CI_2N_2O$	357.32	1.023					
N-benzyl Furanyl norfentanyl	$C_{23}H_{24}N_2O_2$	360.45	1.018					
Cyclobutyl fentanyl	$C_{24}H_{30}N_2O$	362.51	1.015					
ortho-methyl Cyclopropyl fentanyl	$C_{24}H_{30}N_2O$	362.51	1.015					
<i>para</i> -methyl Cyclopropyl fentanyl	$C_{24}H_{30}N_2O$	362.51	1.015					
<i>meta</i> -methyl Cyclopropyl fentanyl	$C_{24}H_{30}N_2O$	362.51	1.015					
Senecioylfentanyl	$C_{24}H_{30}N_2O$	362.51	1.015					
<i>para</i> -methoxy Acrylfentanyl	$C_{23}H_{28}N_2O_2$	364.48	1.013					
(±)- <i>cis</i> -3-methyl Butyryl fentanyl	$C_{24}H_{32}N_2O$	364.52	1.013					
α-methyl Butyryl fentanyl	$C_{24}H_{32}N_2O$	364.52	1.013					
α'-methyl Butyryl fentanyl	$C_{24}H_{32}N_2O$	364.52	1.013					
Isovaleryl fentanyl	$C_{24}H_{32}N_2O$	364.52	1.013					

<i>para</i> -methyl Isobutyryl fentanyl	$C_{24}H_{32}N_2O$	364.52	1.013						
Pivaloyl fentanyl	$C_{24}H_{32}N_2O$	364.52	1.013						
<i>para</i> -methyl Butyryl fentanyl	$C_{24}H_{32}N_2O$	364.52	1.013						
<i>para</i> -fluoro Crotonyl fentanyl	C <sub>23</sub> H <sub>27</sub> FN <sub>2</sub> O	366.47	1.010						
<i>para</i> -fluoro Cyclopropyl fentanyl	C <sub>23</sub> H <sub>27</sub> FN <sub>2</sub> O	366.47	1.010						
para-Methoxyfentanyl	$C_{23}H_{30}N_2O_2$	366.50	1.010					0.986	
ortho-methyl Methoxyacetyl fentanyl	$C_{23}H_{30}N_2O_2$	366.50	1.010						
α'-methoxy Fentanyl	$C_{23}H_{30}N_2O_2$	366.50	1.010						
Ethoxyacetyl fentanyl	$C_{23}H_{30}N_2O_2$	366.50	1.010						
<i>meta</i> -methyl Methoxyacetyl fentanyl	$C_{23}H_{30}N_2O_2$	366.50	1.010						
<i>para</i> -methyl Methoxyacetyl fentanyl	$C_{23}H_{30}N_2O_2$	366.50	1.010						
Ohmefentanyl	$C_{23}H_{30}N_2O_2$	366.50	1.010						
2-fluoro MT-45	$C_{24}H_{31}FN_2$	366.51	1.010						

<i>meta</i> -Fluorobutyryl fentanyl	C <sub>23</sub> H <sub>29</sub> FN <sub>2</sub> O	368.49	1.007					
<i>meta</i> -Fluoroisobutyryl fentanyl	$C_{23}H_{29}FN_2O$	368.49	1.007					
<i>ortho</i> -Fluoroisobutyryl fentanyl	$C_{23}H_{29}FN_2O$	368.49	1.007					
<i>para</i> -Fluorobutyryl fentanyl	$C_{23}H_{29}FN_2O$	368.49	1.007					
para-chloro Acrylfentanyl	C <sub>22</sub> H <sub>25</sub> CIN <sub>2</sub> O	368.90	1.006					
<i>meta</i> -fluoro Methoxyacetyl fentanyl	$C_{22}H_{27}FN_2O_2$	370.46	1.004					
<i>para</i> -fluoro Methoxyacetyl fentanyl	C <sub>22</sub> H <sub>27</sub> FN <sub>2</sub> O <sub>2</sub>	370.46	1.004					
Ocfentanil	C <sub>22</sub> H <sub>27</sub> FN <sub>2</sub> O <sub>2</sub>	370.46	1.004					
para-Chlorofentanyl	C <sub>22</sub> H <sub>27</sub> CIN <sub>2</sub> O	370.92	1.004					
2'-fluoro <i>ortho</i> - Fluorofentanyl	$C_{22}H_{26}F_2N_2O$	372.45	1.002					
Furanyl fentanyl 3- furancarboxamide isomer	$C_{24}H_{26}N_2O_2$	374.47	0.999					
Cyclopentenyl fentanyl	$C_{25}H_{30}N_2O$	374.52	0.999					

N-(3-ethylindole) Norfentanyl	$C_{24}H_{29}N_3O$	375.51	0.998						
Remifentanil	$C_{20}H_{28}N_2O_5$	376.44	0.996						1.005
Mirfentanil	$C_{22}H_{24}N_4O_2$	376.45	0.996						
Cyclopentyl fentanyl	$C_{25}H_{32}N_2O$	376.53	0.996					0.976	
3-Allylfentanyl	$C_{25}H_{32}N_2O$	376.53	0.996						
Tetrahydrofuran fentanyl	$C_{24}H_{30}N_2O_2$	378.51	0.994	0.990					0.985
Hexanoyl fentanyl	$C_{25}H_{34}N_2O$	378.55	0.994						
Benzyl Carfentanil	$C_{23}H_{28}N_2O_3$	380.48	0.991						
<i>para</i> -methoxy Butyryl fentanyl	$C_{24}H_{32}N_2O_2$	380.52	0.991						
ortho-methoxy Butyryl fentanyl	$C_{24}H_{32}N_2O_2$	380.52	0.991					0.960	
4-Methoxymethyl fentanyl	$C_{24}H_{32}N_2O_2$	380.52	0.991						
<i>para</i> -methoxy Methoxyacetyl fentanyl	$C_{23}H_{30}N_2O_3$	382.49	0.989						
<i>para</i> -fluoro Valeryl fentanyl	$C_{24}H_{31}FN_2O$	382.51	0.989						

<i>para</i> -chloro Cyclopropyl fentanyl	C <sub>23</sub> H <sub>27</sub> ClN <sub>2</sub> O	382.93	0.988					
Phenyl fentanyl	$C_{26}H_{28}N_2O$	384.51	0.986				0.980	
<i>para</i> -Chloroisobutyryl fentanyl	$C_{23}H_{29}CIN_2O$	384.94	0.986					
<i>para</i> -Chlorobutyryl fentanyl	C <sub>23</sub> H <sub>29</sub> ClN <sub>2</sub> O	384.94	0.986					
4'-fluoro, para-fluoro (±)- <i>trans</i> -3-methyl Fentanyl	$C_{23}H_{28}F_2N_2O$	386.48	0.984					
Sufentanil	$C_{22}H_{30}N_2O_2S$	386.55	0.984					0.989
<i>para</i> -chloro Methoxyacetyl fentanyl	C <sub>22</sub> H <sub>27</sub> CIN <sub>2</sub> O <sub>2</sub>	386.91	0.984					
<i>ortho</i> -methyl Furanyl fentanyl	$C_{25}H_{28}N_2O_2$	388.50	0.982					
<i>ortho</i> -methyl Furanyl fentanyl	$C_{25}H_{28}N_2O_2$	388.50	0.982				0.980	
<i>meta</i> -methyl Furanyl fentanyl	$C_{25}H_{28}N_2O_2$	388.50	0.982					
<i>para</i> -methyl Furanyl fentanyl	$C_{25}H_{28}N_2O_2$	388.50	0.982					
Cyclohexyl fentanyl	$C_{26}H_{34}N_2O$	390.56	0.980					

<i>para</i> -methyl Cyclopentyl fentanyl	$C_{26}H_{34}N_2O$	390.56	0.980					
<i>ortho</i> -fluoro Furanyl fentanyl	$C_{24}H_{25}FN_2O_2$	392.47	0.977					
<i>para</i> -fluoro Furanyl fentanyl 3- furancarboxamide	$C_{24}H_{25}FN_2O_2$	392.47	0.977					
<i>para</i> -fluoro Furanyl fentanyl	$C_{24}H_{25}FN_2O_2$	392.47	0.977					
<i>para</i> -methyl Tetrahydrofuran fentanyl	$C_{25}H_{32}N_2O_2$	392.53	0.977					
Heptanoyl fentanyl	$C_{26}H_{36}N_2O$	392.58	0.977					
<i>para</i> -fluoro Cyclopentyl fentanyl	$C_{25}H_{31}FN_2O$	394.52	0.975					
<i>para</i> -methoxy Valeryl fentanyl	$C_{25}H_{34}N_2O_2$	394.55	0.975					
Tetrahydrothiophene fentanyl	$C_{24}H_{30}N_2OS$	394.57	0.975					
<i>para</i> -fluoro Tetrahydrofuran fentanyl	$C_{24}H_{29}FN_2O_2$	396.50	0.973					
<i>para</i> -chloro Cyclobutyl fentanyl	$C_{24}H_{29}CIN_2O$	396.95	0.973					

<i>ortho</i> -methyl Phenyl fentanyl	$C_{27}H_{30}N_2O$	398.54	0.971					
Phenylacetyl fentanyl	$C_{27}H_{30}N_2O$	398.54	0.971					
<i>para</i> -chloro Valeryl fentanyl	$C_{24}H_{31}CIN_2O$	398.97	0.971					
<i>para</i> -methoxy Furanyl fentanyl	$C_{25}H_{28}N_2O_3$	404.50	0.965					
<i>ortho</i> -methoxy Furanyl fentanyl	$C_{25}H_{28}N_2O_3$	404.50	0.965				0.960	
2,2,3,3-tetramethyl- Cyclopropyl fentanyl	$C_{27}H_{36}N_2O$	404.59	0.965					
<i>para</i> -methoxy Tetrahydrofuran fentanyl	$C_{25}H_{32}N_2O_3$	408.53	0.962					
Lofentanil	$C_{25}H_{32}N_2O_3$	408.53	0.962					
<i>para</i> -chloro Furanyl fentanyl	$C_{24}H_{25}CIN_2O_2$	408.92	0.961				0.950	
<i>para</i> -chloro Cyclopentyl fentanyl	C <sub>25</sub> H <sub>31</sub> CIN <sub>2</sub> O	410.98	0.959					
β'-Phenyl fentanyl	C <sub>28</sub> H <sub>32</sub> N <sub>2</sub> O	412.57	0.958					
4-Phenyl fentanyl	$C_{28}H_{32}N_2O$	412.57	0.958					
Phenoxyacetyl fentanyl	$C_{27}H_{30}N_2O_2$	414.54	0.956					

Alfentanil	$C_{21}H_{32}N_6O_3$	416.52	0.955					0.945
Thiafentanil	$C_{22}H_{28}N_2O_4S$	416.53	0.955					
<i>ortho</i> -isopropyl Furanyl fentanyl	$C_{27}H_{32}N_2O_2$	416.55	0.955				0.930	
Brifentanil	$C_{20}H_{29}FN_6O_3$	420.48	0.952					
Benzodioxole fentanyl	$C_{27}H_{28}N_2O_3$	428.52	0.946					
Trefentanil	$C_{25}H_{31}FN_6O_2$	466.55	0.930					

# References

[1] H Zaknoun, M Binette, M Tam (2019) Analyzing fentanyl and fentanyl analogues by ion mobility spectrometry, International Journal for Ion Mobility Spectrometry, published online, <u>https://doi.org/10.1007/s12127-019-00244-0</u>.

[2] E Sisco, J R Verkouteren, J Staymates, J Lawrence (2017) Rapid detection of fentanyl, fentanyl analogues, and opioids for on-site or laboratory based drug seizure screening using thermal desorption DART-MS and ion mobility spectrometry, Forensic Chemistry 4, 108-115.

[3] C Ruzicka, FDA, personal communication.

**Table S2.** Instruments used in study identified by model and make and with identifying software version. Details provided on changes to default instrument settings and cleaning procedures following fentanyl and fentanyl-related substance testing. Instruments ordered alphabetically.

# Implant Sciences QS-B220 (s/n 0713-B4D-0080)

- Software: ECAC Configuration, v. 1.2.0 (d=23176)
- Settings Adjustments: Desorber Temp to 235 °C (from 220 °C), Analysis Time to 15.0s (from 12.0s)
- Unadjusted Settings of Note: Nozzle Temp. (Pos.) = 180 °C, Pos. Drift Tube\_0 = 100 °C
- Hardware Adjustments:
- Cleaning Procedures:
  - Interior and exterior of plastic desorber face plate were wiped.
  - Interior and exterior of desorber inlet and outlet were wiped.
  - Desorber filter was replaced.
  - Interior and exterior of the inlets and outlets of both the negative and positive IMS assemblies were wiped.
  - Exhaust filter was removed, and either a new filter will be secured or the old will be after cleaning.
  - Exhaust fan replaced with a new fan.
  - Exhaust cavity was wiped.

## Morpho Itemiser DX (s/n 180982) (internal calibrant modification)

- Software: Narcotics Mode, v. 8.91.2
- Settings Adjustments: None
- Unadjusted Settings of Note: Desorber Temp. = 235 °C, Detector Temp. = 202 °C, Sample Time = 13.0s
- Hardware Adjustments: internal manufacturer-supplied calibrant modification remained in use
- Cleaning Procedures:
  - Wiped interior and exterior of plastic shell near desorber mouth.
  - Wiped desorber mouth and exit of desorber.
  - Replaced filter screen from inlet nozzle and placed contaminated screen aside for analysis.
  - Wiped down inlet assembly.
  - Replaced O-ring at brass inlet.
  - The following tubing sections were removed, and the junctions were wiped before replacing with fresh tubing: IMS outlet to "T" junction, "T" junction to pressure detector, "T" junction to first valve.
  - "T" junction was wiped thoroughly and returned to service.
  - Calibrant cannister was replaced as were the tubing lines that immediately entered and exited the cannister.
  - Rear fan was wiped and filter was replaced.
  - Instrument was placed into a 60-minute system clean.

## Morpho Itemiser DX (s/n 180982) (without internal calibrant)

- Software: Narcotics Mode, v. 8.91.2
- Settings Adjustments: None
- Unadjusted Settings of Note: Desorber Temp. = 235 °C, Detector Temp. = 202 °C, Sample Time = 13.0s
- Hardware Adjustments: internal manufacturer-supplied calibrant modification removed
- Cleaning Procedures: as above

#### Morpho Itemiser 4DX (s/n 241014)

- Software: Exp./Nar. Mode, v. C10.06.7d-COMM (custom), GUI v. 10.09zh
- Settings Adjustments: Detector Temp to 202 °C (from 163 °C)
- Unadjusted Settings of Note: Desorber Temp. = 235 °C, Sample Time = 12.0s, Flow In = 80.0cc/min, Dopant Flow Out = 90.0cc/min
- Hardware Adjustments: filter attached to exhaust port/tubing extension attached to exhaust filter such that exhaust gases would exit into hood
- Cleaning Procedures:
  - Wiped interior and exterior of plastic shell near desorber mouth.
  - Wiped desorber mouth and exit of desorber with as much penetration as possible.
  - Replaced filter screen from inlet nozzle.
  - Wiped down inlet assembly.
  - Replaced O-ring at brass inlet.
  - Removed exhaust tubing, wiped connection junction, and attached the original exhaust tubing.
  - Removed exhaust filter with all attached elbows, wiped connections, and installed fresh tubing.
  - Instrument was placed into a 60-minute thermal clean.

#### Smiths Detection Ionscan 500DT (s/n 52468)

- Software: AE configuration, Rev. L, OS 6.0, Release 500DT\_3.05.022
- Settings Adjustments: Desorber Temperature to 245 °C (from 205 °C), Analysis Time to 15.0s (from 5.0s)
- Unadjusted Settings of Note: Inlet Heater = 285 °C, Drift Heater = 220 °C
- Hardware Adjustments: None
- Cleaning Procedures:
  - Condenser Tubes were replaced
  - Rubber gaskets at condenser tube junctions were replaced and the points of contact were wiped.
  - Preventative maintenance procedures were performed on the inlet assembly: T-tube inlet liner was removed and wiped, interior and exterior of interface block liner assembly were wiped, T-tube and interface block liner gaskets were replaced. Desorber ring seal was replaced and desorber head was wiped.

- Desorber mouth of plastic cover was wiped.
- Notes: Analysis time was extended to improve desorption efficiency. All analyses were performed using NE mode Nomex wipes. Stage 1 Analysis Time = 6.0s (originally 2.0s), Stage 2 Analysis Time = 9.0s (originally 3.0s).

### Smiths Detection Ionscan 500DT (s/n 50152)

- Software: NE configuration, Rev. J, OS 6.0, Release 500DT\_3.05.022
- Settings Adjustments: None
- Unadjusted Settings of Note: Desorber Temp. = 245 °C, Inlet Heater = 265 °C, Drift Heater = 244 °C, Sample Time = 8.0s
- Hardware Adjustments: None
- Cleaning Procedures: see s/n 52468
- Notes: Stage 1 Analysis Time = 2.0s, Stage 2 Analysis Time = 6.0s.

#### Smiths Detection Ionscan 600 (s/n 65472)

- Software: High Temp. Fentanyl Narc. Prelim (25332-D), v. 9824012-K-r.5812, IMS v. 1.72.0.1, Analog v. 1.117.0.2
- Settings Adjustments: None
- Unadjusted Settings of Note: Collector Temp. = 169°C, Inlet Temp. = 181°C, Drift Tube Temp. = 170°C,
- Hardware Adjustments: None
- Cleaning Procedures:
  - Wiped entire interior of <sup>3</sup>/<sub>4</sub> sided plastic shell.
  - Wiped interior and exterior of plastic shell near desorber mouth and vented areas.
  - Wiped both fans near rear of instrument.
  - Removed the following tubes so that tubing ends and junctions could be wiped: 'IMS spl,' 'INL Byp,' 'IMS dft,' 'IMS Exh.' After wiping, the tubes were reconnected.
  - Wiped all observed junction exteriors.
- Notes: Manufacturer recommends company-supplied cleaning.