Propellants, Explosives, Pyrotechnics

Supporting Information

Exploring Rapid, Sensitive and Reliable Detection of Trace Explosives Using Paper Spray Mass Spectrometry (PS-MS)

Catia Costa,* Elsje M. van Es, Patrick Sears, Josephine Bunch, Vladimir Palitsin, Kirsten Mosegaard, and Melanie J. Bailey

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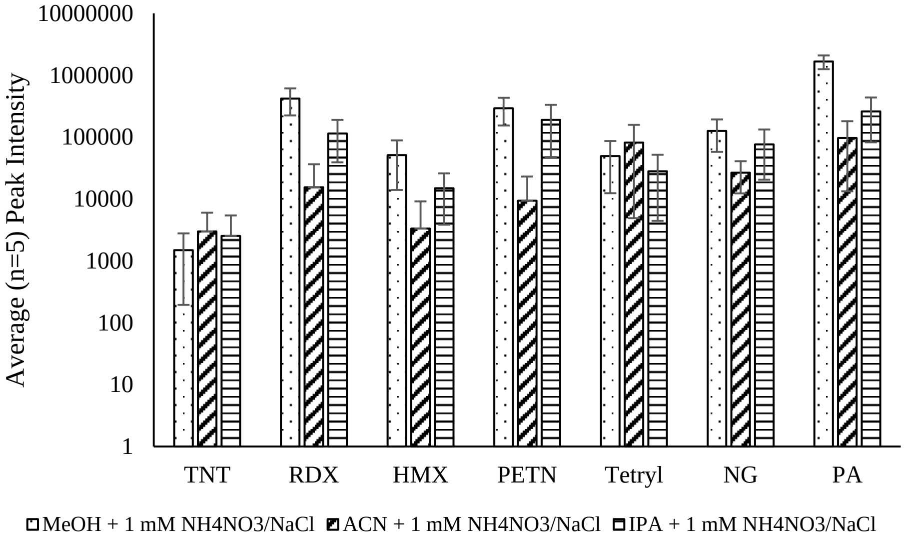
*Ion Beam Centre, University of Surrey, Guildford, Surrey GU2 7XH, UK; c.d.costa@surrey.ac.uk

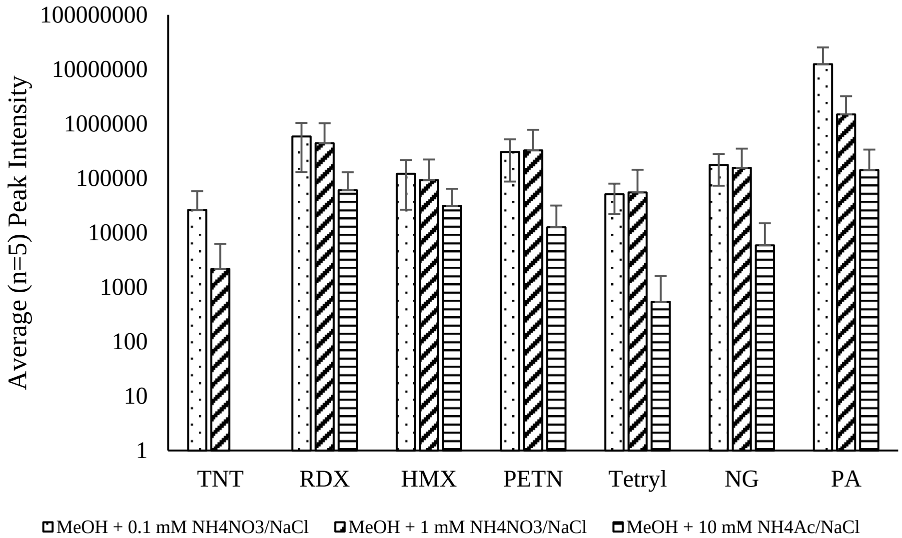
Supplemental Data Table 1 - Target analytes, common adducts formed, respective monoisotopic masses and % of each adduct formed.

Explosive	Adducts Ions	Monoisotopic Mass	%
Trinitrotoluene (TNT)	**$[TNT]^-$**	227.0173	0%
	$[TNT-H]^-$	226.0106	100%
1,3,5-Trinitroperhydro-1,3,5-triazine (RDX)	**$[RDX + {}^{35}Cl]^-$**	257.0043	19%
	$[RDX + {}^{37}Cl]^-$	259.0008	6%
	$[RDX + NO_3]^-$	284.0233	75%
	$[RDX + Ac]^-$	281.0487	0%
Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX)	**$[HMX + {}^{35}Cl]^-$**	331.0159	38%
	$[HMX + {}^{37}Cl]^-$	333.0124	12%
	$[HMX + NO_3]^-$	358.0349	50%
	$[HMX + Ac]^-$	355.0604	0%
Pentaerythritol tetranitrate (PETN)	**$[PETN + {}^{35}Cl]^-$**	350.9833	20%
	$[PETN + {}^{37}Cl]^-$	352.9798	6%
	$[PETN + NO_3]^-$	378.0022	74%
	$[PETN + NO_2]^-$	362.0073	0%
	$[PETN - H]^-$	315.0066	0%
	$[PETN + Ac]^-$	375.0277	0%
Tetryl	**$[Tetryl + {}^{35}Cl]^-$**	321.9832	6%
	$[Tetryl + {}^{37}Cl]^-$	323.9797	1%
	$[Tetryl + NO_3]^-$	349.0022	91%
	$[Tetryl + NO_2]^-$	333.0073	3%
	$[Tetryl + Ac]^-$	241.0215	0%
Nitroglycerin (NG)	**$[NG + {}^{35}Cl]^-$**	261.9720	10%

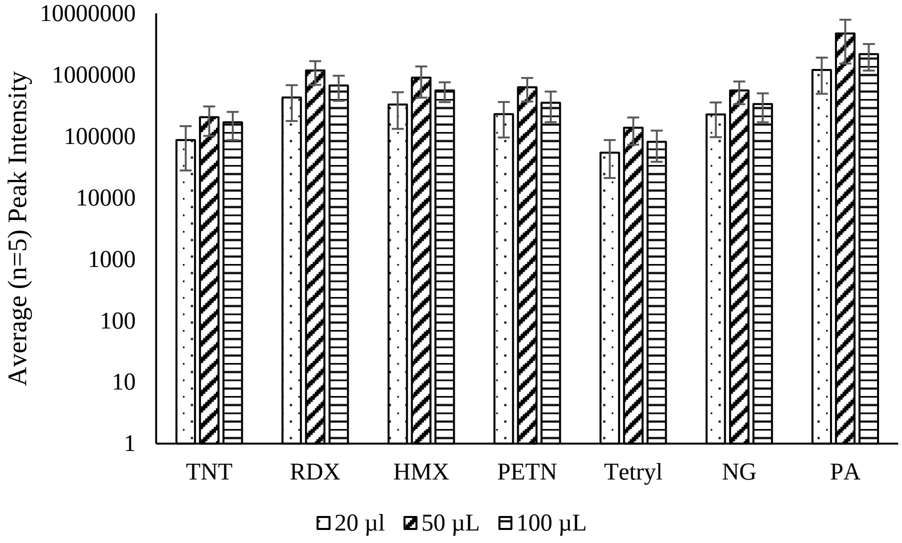
	[NG + ^{37}Cl]$^-$	263.9685	2%
	[NG + NO_3]$^-$	288.9909	87%
	[NG + NO_2]$^-$	272.9960	0%
	[NG - H]$^-$	225.9953	0%
	[NG + Ac]$^-$	286.0164	0%
Picric Acid (PA)	**[PA-H]$^-$**	227.9898	100%
Hexamethylene triperoxide diamine (HMTD)	**[HMTD-H_2+Na]$^+$**	226.0431	100%
Dinitrotoluene (DNT)	**[DNT]$^-$**	184.0490	-
	[DNT - H]$^-$	183.0411	-
Paracetamol (PMOL)	**[PMOL-H]$^-$**	150.0555	-
	[2PMOL-H]$^-$	301.1188	-
	[PMOL+^{35}Cl]$^-$	186.0322	-
	[PMOL+^{37}Cl]$^-$	188.0292	-
	[PMOL+NO_3]$^-$	213.0511	-
Chloramphenicol (CAM)	**[CAM (^{35}Cl ^{35}Cl)]$^-$**	322.0129	0%
	[CAM (^{35}Cl ^{37}Cl)]$^-$	324.0099	0%
	[CAM (^{37}Cl ^{37}Cl)]$^-$	326.0070	0%
	[CAM (^{35}Cl ^{35}Cl) - H]$^-$	321.0051	34%
	[CAM (^{35}Cl ^{37}Cl) - H]$^-$	323.0021	20%
	[CAM (^{37}Cl ^{37}Cl) - H]$^-$	324.9992	3%
	[CAM (^{35}Cl ^{35}Cl) + NO_3]$^-$	384.0007	26%
	[CAM (^{35}Cl ^{37}Cl) + NO_3]$^-$	385.9977	16%
	[CAM (^{37}Cl ^{37}Cl) + NO_3]$^-$	387.9948	2%



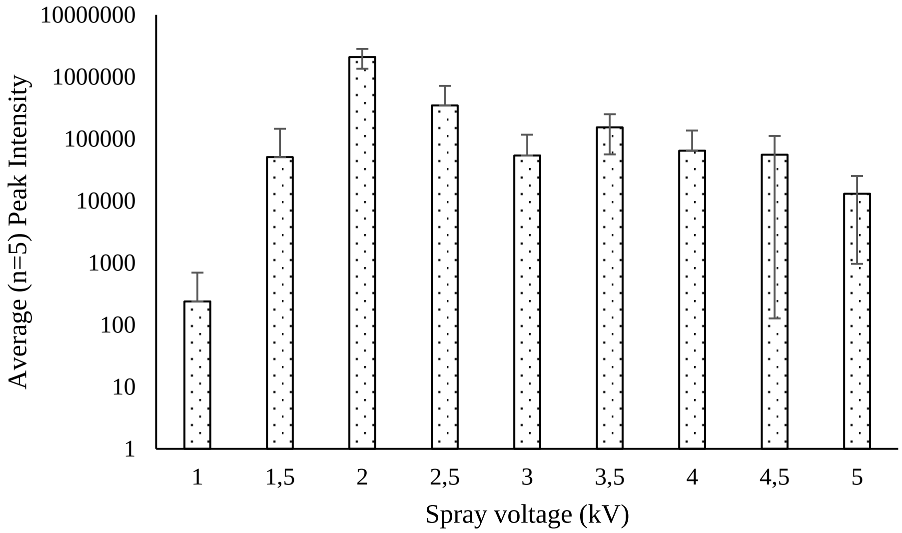
Supplemental Data Figure 1. Average (n=5) peak intensities measured using 100 µL of methanol (MeOH), acetonitrile (ACN) and isopropanol (IPA) with 1 mM NH_4NO_3/NaCl as spray solvents for the detection of explosives in negative ion mode using paper spray mass spectrometry



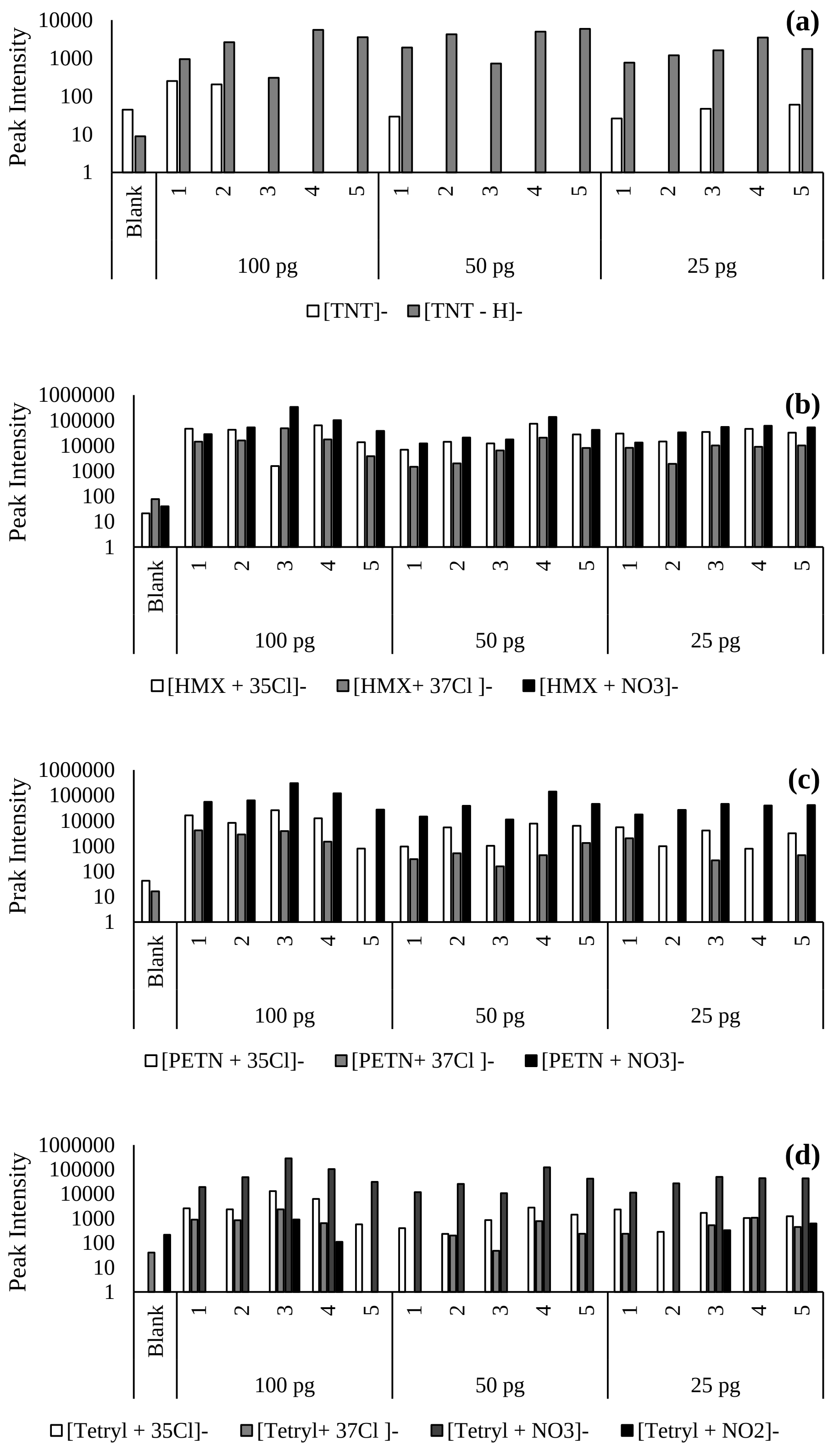
Supplemental Data Figure 2. Average (n=5) peak intensities measured using 100 µL of methanol (MeOH) with 0.1 mM NH_4NO_3/NaCl, 1 mM NH_4NO_3/NaCl and 10 mM NH_4Ac/NaCl as spray solvent additives for the detection of explosives in negative ion mode using paper spray mass spectrometry

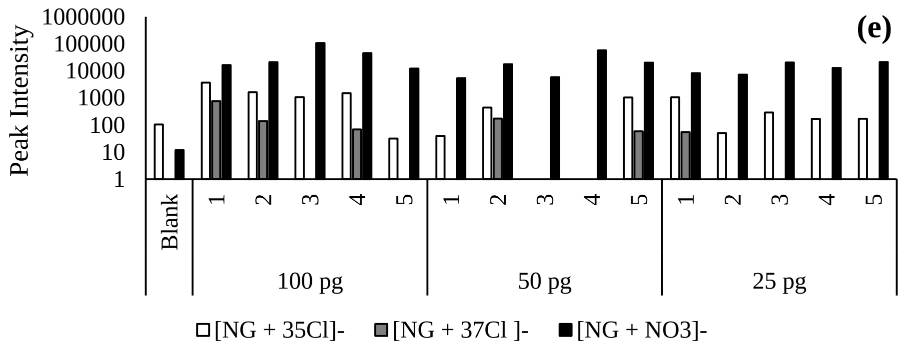


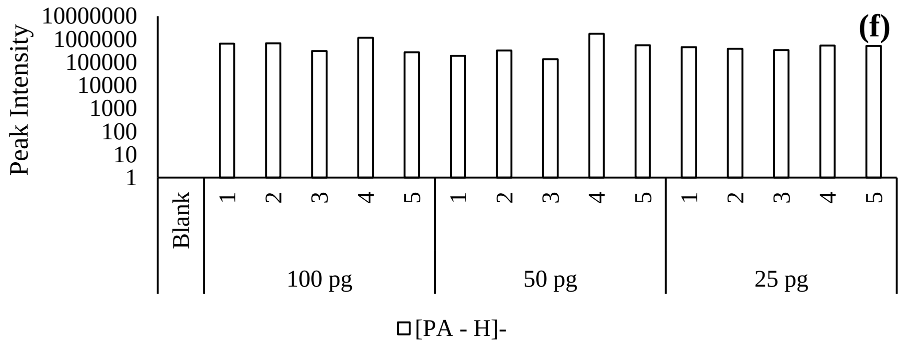
Supplemental Data Figure 3. Average (n=5) peak intensities measured using 20, 50 and 100 µL of methanol (MeOH) with 0.1 mM NH_4NO_3/NaCl for the detection of explosives in negative ion mode using paper spray mass spectrometry



Supplemental Data Figure 4. Average (n=5) peak intensities measured using 100 µL of methanol (MeOH) with 0.1 mM NH_4NO_3/NaCl at increasing spray voltages for the detection of explosives in negative ion mode using paper spray mass spectrometry


(a)
Peak Intensity
10000
1000
100
10
1
Blank
1 2 3 4 5
100 pg
50 pg
25 pg
[TNT]-
[TNT - H]-
(b)
Peak Intensity
1000000
100000
10000
1000
100
10
1
[HMX + 35Cl]-
[HMX+ 37Cl]-
[HMX + NO3]-
(c)
Prak Intensity
[PETN + 35Cl]-
[PETN+ 37Cl]-
[PETN + NO3]-
(d)
Peak Intensity
[Tetryl + 35Cl]-
[Tetryl+ 37Cl]-
[Tetryl + NO3]-
[Tetryl + NO2]-





Supplemental Data Figure 5. Measured peak intensities for (top to bottom) (a) TNT, (b) HMX, (c) PETN, (d) tetryl, (e) NG and (f) PA at 25, 50 and 100 pg measured using the paper spray method developed for the detection of explosives in negative ion mode