

Supplementary Data

Solid-phase extraction using hierarchical organosilicates for enhanced detection of nitroenergetic targets

Brandy J. Johnson^{1*}, Brian J. Melde¹, Iwona A. Leska², Paul T. Charles¹, Alan D. Hewitt³

¹Center for Bio/Molecular Science and Engineering, Naval Research Laboratory, Washington, DC; ²NOVA Research Incorporated, Alexandria, VA; ³Engineer Research and Development Center, US Army Corps of Engineers, NH

*brandy.white@nrl.navy.mil, fax: 202 404 8897

The supplementary data supplied here provides materials characterization for the MM1 organosilicate material, Sep-Pak, and LiChrolut EN. Also included are complete results of HPLC analysis for extraction of 2,4,6-trinitrotoluene (TNT), 2,4-dinitrotoluene (DNT), nitroglycerine (NG), 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX), and octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocane (HMX) from deionized water, artificial sea water, groundwater, surface water, and soil sample extracts.

Figure S1. Characterization of materials. Shown here are the nitrogen sorption isotherms and pore size distributions for each of the three materials: MM1 (circle), Sep-Pak (square; data shifted by +450), and LiChrolut EN (diamond). A table of material characteristics is also provided.

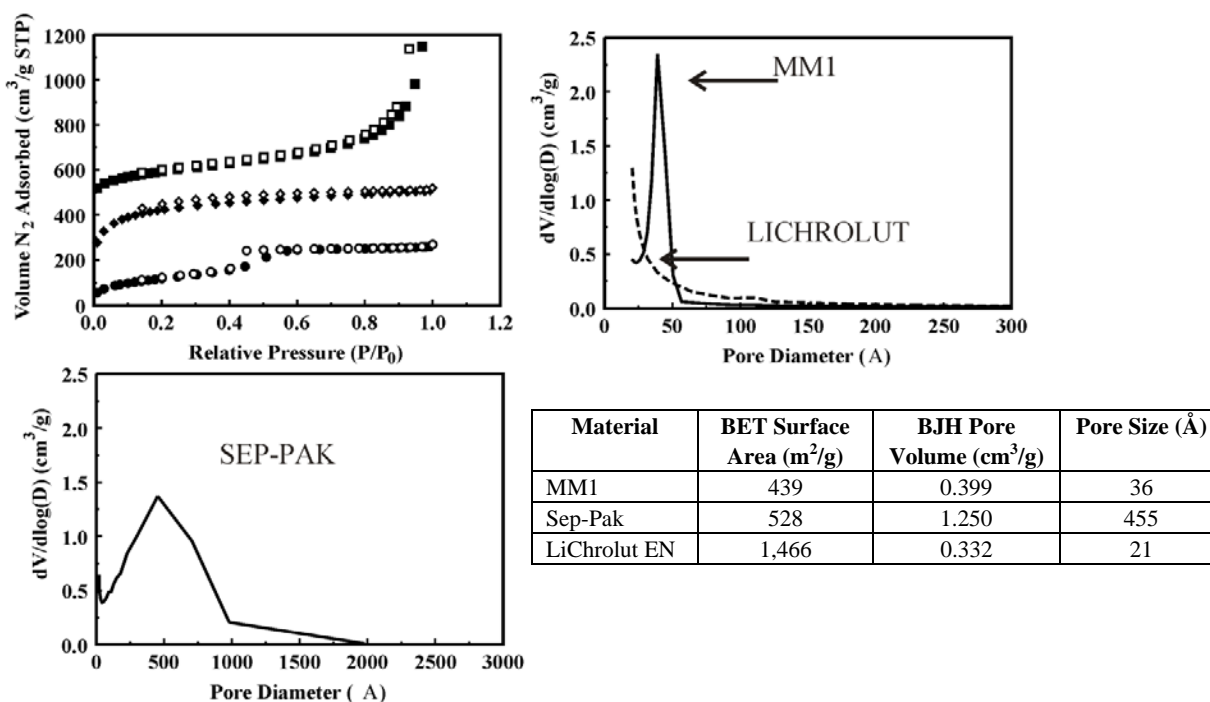


Table S1. Deionized Water. Shown here are the results of HPLC analysis of samples containing a single nitroenergetic target at varying concentrations in deionized water. “Flow through” indicates the column effluent during sample exposure (20 mL). “Water rinse” indicates column flush using deionized water (6 mL). “ACN flush” indicates elution of targets using acetonitrile (4 mL). ND (not detected) is used to denote levels below the detection limit for the analytical method. Data is provided as concentrations in parts per billion, in total micrograms recovered, and as a percentage of the total applied target. Three-sigma variations for these experiments are between 7 and 11%.

		MM1			Sep-Pak			LiChrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
TNT 200 ppb 4.0 µg	Flow through	ND	ND	ND	38	0.76	19	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	848	3.39	85	706	2.82	71	850	3.40	85
	ACN flush 2	21	0.08	2	86	0.34	9	126	0.50	13
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
TNT 50 ppb 1.0 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	219	0.87	88	187	0.75	75	245	0.98	99
	ACN flush 2	ND	ND	ND	27	0.11	11	0	0.00	0
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
TNT 5 ppb 0.1 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	24	0.10	97	22	0.09	88	25	0.10	101
	ACN flush 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
TNT 0.9 ppb 0.02 µg	All volumes	ND	ND	ND	ND	ND	ND	ND	ND	ND
		MM1			Sep-Pak			Lichrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
RDX 198 ppb 4.0 µg	Flow through	ND	ND	ND	67	1.33	33	ND	ND	ND
	Water rinse 1	ND	ND	ND	25	0.15	4	10	0.06	1
	ACN flush 1	915	3.66	92	590	2.36	59	992	3.97	99
	ACN flush 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
RDX 50 ppb 1.0 µg	Flow through	ND	ND	ND	28	0.55	56	ND	ND	ND
	Water rinse 1	ND	ND	ND	22	0.13	13	ND	ND	ND
	ACN flush 1	237	0.95	94	146	0.59	59	217	0.87	88
	ACN flush 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
RDX 5 ppb 0.1 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	24	0.10	96	ND	ND	ND	ND	ND	ND
	ACN flush 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
RDX 0.9 ppb 0.02 µg	All volumes	ND	ND	ND	ND	ND	ND	ND	ND	ND

Table S1. (deionized water continued)

		MM1			Sep-Pak			Lichrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
HMX 197 ppb 3.9 µg	Flow through	ND	ND	ND	51	1.02	25	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	784	3.14	78	524	2.10	52	529	2.12	53
	ACN flush 2	ND	ND	ND	40	0.16	4	112	0.45	11
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
HMX 53 ppb 1.0 µg	Flow through	ND	ND	ND	19	0.37	37	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	198	0.79	79	110	0.44	44	126	0.51	51
	ACN flush 2	ND	ND	ND	19	0.08	8	35	0.14	14
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
HMX 5 ppb 0.1 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	ND	ND	ND	ND	ND	ND	14	0.06	56
	ACN flush 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
HMX 0.9 ppb 0.02 µg	All volumes	ND	ND	ND	ND	ND	ND	ND	ND	ND
		MM1			Sep-Pak			Lichrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
DNT 200 ppb 4.0 µg	Flow through	ND	ND	ND	41	0.81	20	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	731	2.92	91	733	2.93	73	729	2.92	95
	ACN flush 2	ND	ND	ND	139	0.56	14	92	0.37	12
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
DNT 50 ppb 1.0 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	223	0.89	89	171	0.69	69	241	0.96	97
	ACN flush 2	ND	ND	ND	58	0.23	23	32	0.13	13
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
DNT 5 ppb 0.1 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	22	0.09	90	16	0.06	65	16	0.07	87
	ACN flush 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
DNT 0.9 ppb 0.02 µg	All Volumes	ND	ND	ND	ND	ND	ND	ND	ND	ND

Table S1. (deionized water continued)

		MM1			Sep-Pak			Lichrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
NG 200 ppb 4.0 µg	Flow through	ND	ND	ND	4	0.08	2	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	727	2.91	87	589	2.35	57	766	3.06	74
	ACN flush 2	ND	ND	ND	99	0.40	10	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
NG 50 ppb 1.0 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	137	0.55	91	77	0.31	51	227	0.91	76
	ACN flush 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
NG 5 ppb 0.10 µg	All volumes	ND	ND	ND	ND	ND	ND	ND	ND	ND
NG 0.9 ppb 0.02 µg	All volumes	ND	ND	ND	ND	ND	ND	ND	ND	ND

Table S2. Artificial Sea Water. Shown here are the results of HPLC analysis of samples containing a single nitroenergetic target at varying concentrations in artificial sea water. “Flow through” indicates the column effluent during sample exposure (20 mL). “Water rinse” indicates column flush using deionized water (6 mL). “ACN flush” indicates elution of targets using acetonitrile (4 mL). ND (not detected) is used to denote levels below the detection limit for the analytical method. Data is provided as concentrations in parts per billion, in total micrograms recovered, and as a percentage of the total applied target.

		MM1			Sep-Pak			LiChrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
TNT 200 ppb 4.0 µg	Flow through	ND	ND	ND	25	0.50	12	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	897	3.59	90	811	3.24	81	782	3.13	78
	ACN flush 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
TNT 50 ppb 1.0 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	211	0.84	84	207	0.83	82	190	0.76	76
	ACN flush 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
TNT 5 ppb 0.1 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	18	0.07	72	17	0.07	68	23	0.09	93
	ACN flush 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
TNT 0.9 ppb 0.02 µg	All volumes	ND	ND	ND	ND	ND	ND	ND	ND	ND

Table S2. (sea water continued)

		MM1			Sep-Pak			Lichrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
RDX 200 ppb 4.0 µg	Flow through	ND	ND	ND	15	0.31	8	ND	ND	ND
	Water rinse 1	55	0.33	8	ND	ND	ND	ND	ND	ND
	ACN flush 1	852	3.41	85	729	2.91	73	865	3.46	86
	ACN flush 2	ND	ND	ND	ND	ND	ND	91	0.37	9
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
RDX 50 ppb 1.0 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	209	0.84	84	157	0.63	63	215	0.86	86
	ACN flush 2	ND	ND	ND	27	0.11	11	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
RDX 5 ppb 0.1 mg	All volumes	ND	ND	ND	ND	ND	ND	ND	ND	ND
RDX 0.9 ppb 0.02 µg	All volumes	ND	ND	ND	ND	ND	ND	ND	ND	ND
		MM1			Sep-Pak			Lichrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
HMX 200 ppb 4.0 µg	Flow through	19	0.39	10	ND	ND	ND	ND	ND	ND
	Water rinse 1	28	0.17	4	ND	ND	ND	ND	ND	ND
	ACN flush 1	778	3.11	78	508	2.03	51	558	2.23	56
	ACN flush 2	ND	ND	ND	ND	ND	ND	53	0.21	5
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
HMX 50 ppb 1.0 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	185	0.74	74	116	0.46	47	142	0.57	57
	ACN flush 2	ND	ND	ND	ND	ND	ND	19	0.08	8
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
HMX 5 ppb 0.1 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	17	0.07	67	ND	ND	ND	13	0.05	52
	ACN flush 2	ND	ND	ND	ND	ND	ND	7	0.03	30
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
HMX 0.9 ppb 0.02 µg	All volumes	ND	ND	ND	ND	ND	ND	ND	ND	ND

Table S2. (sea water continued)

		MM1			Sep-Pak			Lichrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
DNT 200 ppb 4.0 µg	Flow through	ND	ND	ND	41	0.83	21	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	946	3.78	94	791	3.16	79	810	3.24	81
	ACN flush 2	ND	ND	ND	134	0.54	13	104	0.41	10
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
DNT 50 ppb 1.0 µg	Flow through	ND	ND	ND	12	0.23	23	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	235	0.94	94	196	0.78	78	171	0.68	68
	ACN flush 2	ND	ND	ND	72	0.29	29	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
DNT 5 ppb 0.1 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	20	0.08	81	ND	ND	ND	ND	ND	ND
	ACN flush 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
DNT 0.9 ppb 0.02 µg	All Volumes	ND	ND	ND	ND	ND	ND	ND	ND	ND
		MM1			Sep-Pak			Lichrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
NG 200 ppb 4.0 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	647	2.59	63	422	1.69	41	386	1.54	37
	ACN flush 2	98	0.39	9	ND	ND	ND	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
NG 50 ppb 1.0 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	165	0.66	66	81	0.33	33	78	0.31	31
	ACN flush 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
NG 5 ppb 0.10 µg	All volumes	ND	ND	ND	ND	ND	ND	ND	ND	ND
NG 0.9 ppb 0.02 µg	All volumes	ND	ND	ND	ND	ND	ND	ND	ND	ND

Table S3. Ground Water. Shown here are the results of HPLC analysis of samples containing a single nitroenergetic target at varying concentrations in ground water. “Flow through” indicates the column effluent during sample exposure (20 mL). “Water rinse” indicates column flush using deionized water (6 mL). “ACN flush” indicates elution of targets using acetonitrile (4 mL). ND (not detected) is used to denote levels below the detection limit for the analytical method. Data is provided as concentrations in parts per billion, in total micrograms recovered, and as a percentage of the total applied target.

		MM1			Sep-Pak			Lichrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
TNT 200 ppb 4.0 µg	Flow through	ND	ND	ND	35	0.70	18	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	873	3.49	87	479	1.92	48	567	2.27	57
	ACN flush 2	ND	ND	ND	48	0.19	5	22	0.09	2
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
TNT 50 ppb 1.0 µg	Flow through	ND	ND	ND	18	0.37	37	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	230	0.92	92	114	0.46	46	149	0.59	60
	ACN flush 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
		MM1			Sep-Pak			Lichrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
RDX 200 ppb 4.0 µg	Flow through	ND	ND	ND	21	0.42	10	ND	ND	ND
	Water rinse 1	ND	ND	ND	3	0.02	< 1	ND	ND	ND
	ACN flush 1	924	3.70	92	639	2.55	64	812	3.25	81
	ACN flush 2	ND	ND	ND	14	0.06	1	30	0.12	3
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
RDX 50 ppb 1.0 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	227	0.91	90	127	0.51	50	179	0.72	71
	ACN flush 2	ND	ND	ND	ND	ND	ND	10	0.04	4
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
		MM1			Sep-Pak			Lichrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
DNT 200 ppb 4.0 µg	Flow through	ND	ND	ND	19	0.39	10	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	909	3.64	91	588	2.35	59	716	2.86	71
	ACN flush 2	ND	ND	ND	149	0.60	15	58	0.23	6
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
DNT 49 ppb 1.0 µg	Flow through	ND	ND	ND	8	0.17	17	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	219	0.87	88	156	0.62	63	182	0.73	73
	ACN flush 2	ND	ND	ND	24	0.10	10	18	0.07	7
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND

Table S3. (ground water continued)

		MM1			Sep-Pak			Lichrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
HMX 200 ppb 4.0 µg	Flow through	ND	ND	ND	33	0.66	17	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	23	0.14	3	513	2.05	51	411	1.64	41
	ACN flush 2	672	2.69	67	66	0.26	7	95	0.38	9
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
HMX 49 ppb 1.0 µg	Flow through	ND	ND	ND	20	0.41	41	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	ND	ND	ND	92	0.37	37	112	0.45	44
	ACN flush 2	ND	ND	ND	18	0.07	7	25	0.10	10
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
		MM1			Sep-Pak			Lichrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
NG 201 ppb 4.0 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	861	3.45	86	414	1.65	41	514	2.06	51
	ACN flush 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
NG 48 ppb 1.0 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	186	0.74	74	126	0.50	50	148	0.59	59
	ACN flush 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND

Table S4. Surface Water. Shown here are the results of HPLC analysis of samples containing a single nitroenergetic target at varying concentrations in surface water. “Flow through” indicates the column effluent during sample exposure (20 mL). “Water rinse” indicates column flush using deionized water (6 mL). “ACN flush” indicates elution of targets using acetonitrile (4 mL). ND (not detected) is used to denote levels below the detection limit for the analytical method. Data is provided as concentrations in parts per billion, in total micrograms recovered, and as a percentage of the total applied target.

		MM1			Sep-Pak			Lichrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
TNT 200 ppb 4.0 µg	Flow through	ND	ND	ND	29	0.59	15	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	887	3.55	89	462	1.85	46	520	2.08	52
	ACN flush 2	ND	ND	ND	47	0.19	5	29	0.12	3
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
TNT 50 ppb 1.0 µg	Flow through	ND	ND	ND	20	0.39	39	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	217	0.87	87	157	0.63	63	208	0.83	83
	ACN flush 2	ND	ND	ND	26	0.10	10	20	0.08	8
	Water rinse 2	ND	ND	ND	19	0.12	12	ND	ND	ND

Table S4. (surface water continued)

		MM1			Sep-Pak			Lichrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
RDX 200 ppb 4.0 µg	Flow through	ND	ND	ND	13	0.26	7	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	887	3.55	89	516	2.06	52	819	3.28	82
	ACN flush 2	5	0.02	1	65	0.26	7	48	0.19	5
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
RDX 50 ppb 1.0 µg	Flow through	ND	ND	ND	11	0.22	22	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	210	0.84	84	159	0.64	63	227	0.91	90
	ACN flush 2	ND	ND	ND	13	0.05	5	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
		MM1			Sep-Pak			Lichrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
DNT 202 ppb 4.0 µg	Flow through	ND	ND	ND	33	0.66	17	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	885	3.54	89	715	2.86	72	867	3.47	87
	ACN flush 2	13	0.05	1	136	0.54	14	55	0.22	5
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
DNT 50 ppb 1.0 µg	Flow through	ND	ND	ND	10	0.20	20	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	215	0.86	87	176	0.70	71	222	0.89	89
	ACN flush 2	ND	ND	ND	33	0.13	13	21	0.09	9
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
		MM1			Sep-Pak			Lichrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
HMX 204 ppb 4.1 µg	Flow through	ND	ND	ND	55	1.10	28	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	550	2.20	55	493	1.97	49	613	2.45	61
	ACN flush 2	ND	ND	ND	46	0.18	5	77	0.31	8
	Water rinse 2	ND	ND	ND	ND	ND	ND	28	0.17	4
HMX 50 ppb 1.0 µg	Flow through	ND	ND	ND	37	0.74	73	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	127	0.51	50	77	0.31	30	130	0.52	51
	ACN flush 2	ND	ND	ND	ND	ND	ND	56	0.23	22
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
		MM1			Sep-Pak			Lichrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
NG 198 ppb 4.0 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	808	3.23	81	586	2.34	59	597	2.39	60
	ACN flush 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
NG 50 ppb 1.0 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	212	0.85	85	131	0.53	53	135	0.54	54

	ACN flush 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND

Table S5. Varying pH. Shown here are the results of HPLC analysis of samples of varying pH containing a single nitroenergetic target. “Flow through” indicates the column effluent during sample exposure (20 mL). “Water rinse” indicates column flush using deionized water (6 mL). “ACN flush” indicates elution of targets using acetonitrile (4 mL). ND (not detected) is used to denote levels below the detection limit for the analytical method. Data is provided as concentrations in parts per billion, in total micrograms recovered, and as a percentage of the total applied target.

		MM1			Sep-Pak			Lichrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
TNT pH 3 200 ppb 4.0 µg	Flow through	ND	ND	ND	48	0.97	24	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	773	3.09	77	436	1.74	44	604	2.42	60
	ACN flush 2	ND	ND	ND	98	0.39	10	72	0.29	7
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
TNT pH 3 50 ppb 1.0 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	175	0.70	70	128	0.51	51	140	0.56	56
	ACN flush 2	ND	ND	ND	35	0.14	14	27	0.11	11
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
TNT pH 9 200 ppb 4.0 µg	Flow through	ND	ND	ND	50	1.00	25	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	839	3.36	84	737	2.95	73	684	2.74	68
	ACN flush 2	131	0.52	13	131	0.52	13	81	0.33	8
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
TNT pH 9 50 ppb 1.0 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	214	0.86	85	148	0.59	59	155	0.62	62
	ACN flush 2	ND	ND	ND	32	0.13	13	31	0.12	12
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
		MM1			Sep-Pak			Lichrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
RDX pH 3 200 ppb 4.0 µg	Flow through	ND	ND	ND	35	0.70	18	ND	ND	ND
	Water rinse 1	1	0.01	< 1	ND	ND	ND	ND	ND	ND
	ACN flush 1	860	3.44	86	580	2.32	58	738	2.95	74
	ACN flush 2	ND	ND	ND	5	0.02	< 1	37	0.15	4
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
RDX pH 3 50 ppb 1.0 µg	Flow through	ND	ND	ND	2	0.05	5	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	212	0.85	86	137	0.55	55	157	0.63	63
	ACN flush 2	ND	ND	ND	8	0.03	3	8	0.03	3
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
RDX pH 9 200 ppb 4.0 µg	Flow through	ND	ND	ND	15	0.29	7	ND	ND	ND
	Water rinse 1	ND	ND	ND	3	0.02	< 1	ND	ND	ND
	ACN flush 1	969	3.87	97	634	2.54	64	801	3.20	80
	ACN flush 2	ND	ND	ND	ND	ND	ND	18	0.07	2
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
RDX pH 9 50 ppb 1.0 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	237	0.95	96	146	0.59	59	207	0.83	84
	ACN flush 2	ND	ND	ND	13	0.05	5	4	0.02	2
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND

		MM1			Sep-Pak			Lichrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
DNT pH 3 198 ppb 4.0 µg	Flow through	ND	ND	ND	35	0.70	17	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	878	3.51	88	559	2.24	56	659	2.64	66
	ACN flush 2	14	0.06	1	137	0.55	14	71	0.29	7
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
DNT pH 3 50 ppb 1.0 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	217	0.87	87	128	0.51	51	147	0.59	59
	ACN flush 2	ND	ND	ND	29	0.11	11	22	0.09	9
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
DNT pH 9 198 ppb 4.0 µg	Flow through	ND	ND	ND	32	0.65	16	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	913	3.65	91	747	2.99	74	828	3.31	83
	ACN flush 2	16	0.07	2	153	0.61	15	74	0.30	7
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
DNT pH 9 50 ppb 1.0 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	230	0.92	80	185	0.74	64	229	0.92	80
	ACN flush 2	ND	ND	ND	43	0.17	15	27	0.11	9
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND

Table S5. (pH continued)

		MM1			Sep-Pak			Lichrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
HMX pH 3 200 ppb 4.0 µg	Flow through	ND	ND	ND	68	1.36	34	ND	ND	ND
	Water rinse 1	17	0.10	3	15	0.09	2	ND	ND	ND
	ACN flush 1	671	2.69	67	512	2.05	51	647	2.59	65
	ACN flush 2	ND	ND	ND	53	0.21	5	103	0.41	10
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
HMX pH 3 50 ppb 1.0 µg	Flow through	ND	ND	ND	16	0.31	31	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	151	0.60	61	113	0.45	45	104	0.42	42
	ACN flush 2	ND	ND	ND	16	0.06	6	28	0.11	11
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
HMX pH 9 200 ppb 4.0 µg	Flow through	ND	ND	ND	69	1.37	20	ND	ND	ND
	Water rinse 1	32	0.19	3	ND	ND	ND	ND	ND	ND
	ACN flush 1	1163	4.65	69	717	2.87	42	966	3.86	57
	ACN flush 2	ND	ND	ND	129	0.52	8	147	0.59	9
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
HMX pH 9 49 ppb 0.98 µg	Flow through	ND	ND	ND	19	0.39	22	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	295	1.18	68	176	0.71	41	255	1.02	59
	ACN flush 2	ND	ND	ND	20	0.08	5	45	0.18	10
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND

Table S5. (pH continued)

		MM1			Sep-Pak			Lichrolut EN		
		[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered	[Target] (ppb)	Target (µg)	% recovered
NG pH 3 200 ppb 4.0 µg	Flow through	ND	ND	ND	117	2.34	58	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	631	2.52	63	388	1.55	39	394	1.57	39
	ACN flush 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
NG pH 3 50 ppb 1.0 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	138	0.55	55	110	0.44	44	117	0.47	47
	ACN flush 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
NG pH 9 200 ppb 4.0 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	632	2.53	63	539	2.16	54	562	2.25	56
	ACN flush 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
NG pH 9 50 ppb 1.0 µg	Flow through	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 1	ND	ND	ND	ND	ND	ND	ND	ND	ND
	ACN flush 1	163	0.65	65	125	0.50	50	155	0.62	62
	ACN flush 2	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Water rinse 2	ND	ND	ND	ND	ND	ND	ND	ND	ND

Table S6. Results of analysis of soil samples from sites on Holloman Air Force Base, Alamogordo, NM using EPA Method 8330B provided by Cold Regions Research and Engineering Laboratory, Engineer Research and Development Center, US Army Corps of Engineers. ND is used to denote levels below the detection limit for the analytical method. Concentrations are provided as parts per million under the sample conditions applied in this study.

Sample Identification and Description			Target (ppm)								
			HMX	RDX	TNB	DNB	TNT	2-ADN T	4-ADN T	2,4-DNT	DNA
HO-001	Old 2,000-lb crater		ND	ND	0.01	ND	0.14	0.03	0.04	0.01	ND
HO-004	Old 2,000-lb crater		ND	0.01	0.03	ND	0.05	0.02	0.02	ND	0.01
HO-006	Old 500-lb crater		ND	0.01	ND	ND	ND	0.10	ND	ND	ND
HO-018	Low order bomb crater	Hot Grid	ND	ND	0.01	ND	0.15	ND	0.04	ND	ND
HO-019	Low order bomb crater	Hot Grid	ND	ND	0.01	ND	0.54	0.04	0.01	ND	ND
HO-020	Low order bomb crater	Hot Grid	ND	ND	ND	ND	2.02	0.05	0.04	ND	ND
HO-022	2,000-lb crater	Hot Grid	ND	0.25	0.03	ND	12.50	0.11	0.11	ND	ND
HO-023	2,000-lb crater	Hot Grid	ND	0.04	0.03	ND	2.60	0.12	0.09	0.08	ND
HO-024	2,000-lb crater	Hot Grid	ND	0.01	0.01	ND	2.70	0.12	0.11	ND	ND
HO-025	No visible low-order debris	Cold Grid	ND	ND	0.08	ND	0.58	ND	ND	ND	ND
HO-026	No visible low-order debris	Cold Grid	0.01	ND	0.03	ND	0.19	0.06	ND	ND	0.01
HO-027	No visible low-order debris	Cold Grid	ND	0.02	0.02	ND	0.08	0.11	0.03	0.01	ND

Table S7. Results of analysis of soil samples using MM1 for solid-phase extraction (25 mg sorbent column). Target concentrations are provided for the aqueous extract of the sample (as extracted), the effluent from the column during sample application (effluent), and the concentrated extract from the column (eluate). ND is used to denote levels below the detection limit for the analytical method. Concentrations are provided as parts per million in the respective sample (2 grams soil in 20 mL deionized water).

Target	Sample	HO-001	HO-004	HO-006	HO-018	HO-019	HO-020	HO-022	HO-023	HO-024	HO-025	HO-026	HO-027
2,4-DNT	As Extracted	0.01	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Effluent	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Eluate	0.33	ND	ND	ND	ND	0.06	ND	<0.01	ND	ND	ND	<0.01
2-ADNT	As Extracted	0.01	ND	ND	ND	0.03	0.02	ND	ND	ND	ND	ND	ND
	Effluent	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Eluate	0.29	0.01	0.01	ND	0.43	0.50	0.09	0.08	0.07	0.02	0.01	0.01
4-ADNT	As Extracted	0.02	ND	ND	<0.01	ND	ND	ND	ND	ND	ND	ND	ND
	Effluent	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Eluate	0.35	0.24	ND	0.92	0.50	0.63	0.09	0.01	0.03	ND	ND	ND
DNB	As Extracted	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Effluent	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Eluate	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
HMX	As Extracted	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Effluent	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Eluate	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
RDX	As Extracted	1.32	<0.01	<0.01	ND	ND	ND	<0.01	ND	<0.01	ND	ND	<0.01
	Effluent	0.80	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Eluate	5.23	0.07	0.07	ND	ND	ND	0.22	<0.01	<0.01	ND	ND	<0.01
TNB	As Extracted	0.48	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Effluent	0.21	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND
	Eluate	3.30	0.01	ND	<0.01	0.13	0.10	<0.01	<0.01	ND	ND	ND	ND
TNT	As Extracted	6.59	0.29	ND	0.64	0.59	1.12	0.71	0.10	0.11	ND	ND	ND
	Effluent	1.73	<0.01	ND	0.04	ND	0.02	0.06	ND	ND	ND	ND	ND
	Eluate	54.59	2.87	ND	6.76	5.06	11.94	6.69	1.67	1.51	0.10	0.01	<0.01

Table S8. Results of analysis of soil sample HO-022 using MM1, LiChrolut EN and Sep-Pak for solid-phase extraction (200 mg sorbent column). “Flow through” indicates the column effluent during sample exposure (20 mL). “Water rinse” indicates column flush using deionized water (6 mL). “ACN flush” indicates elution of targets using acetonitrile (4 mL). ND (not detected) is used to denote levels below the detection limit for the analytical method. Concentrations are provided as parts per billion in the respective sample.

Target	Method 8330B	NRL Extraction Protocol		MM1	LiChrolut	Sep-Pak
2,4-DNT	ND	ND	Flow through	ND	ND	ND
			Water rinse 1	ND	ND	ND
			ACN flush 1	ND	ND	ND
			ACN flush 2	ND	ND	ND
			Water rinse 2	ND	ND	ND
2-ADNT	110	16	Flow through	ND	ND	ND
			Water rinse 1	ND	ND	ND
			ACN flush 1	84	72	39
			ACN flush 2	ND	ND	11
			Water rinse 2	ND	ND	ND
4-ADNT	110	68	Flow through	ND	ND	ND
			Water rinse 1	ND	ND	ND
			ACN flush 1	679	689	398
			ACN flush 2	ND	ND	87
			Water rinse 2	ND	ND	4
DNB	ND	ND	Flow through	ND	ND	ND
			Water rinse 1	ND	ND	ND
			ACN flush 1	ND	ND	ND
			ACN flush 2	ND	ND	ND
			Water rinse 2	ND	ND	ND
HMX	ND	ND	Flow through	ND	ND	ND
			Water rinse 1	ND	ND	ND
			ACN flush 1	ND	ND	ND
			ACN flush 2	ND	ND	ND
			Water rinse 2	ND	ND	ND
RDX	250	27	Flow through	ND	ND	12
			Water rinse 1	ND	ND	ND
			ACN flush 1	127	36	21
			ACN flush 2	ND	ND	12
			Water rinse 2	ND	ND	ND
TNB	30	8	Flow through	ND	ND	ND
			Water rinse 1	ND	ND	ND
			ACN flush 1	17	ND	ND
			ACN flush 2	ND	ND	ND
			Water rinse 2	ND	ND	ND
TNT	1250	386	Flow through	ND	ND	90
			Water rinse 1	ND	ND	3
			ACN flush 1	2950	2371	1789
			ACN flush 2	19	443	419
			Water rinse 2	ND	ND	ND