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Supplemental Material

A Method for Identifying Prevalent Chemical Combinations in the U.S. Population

Dustin F. Kapraun, John F. Wambaugh, Rogelio Tornero-Velez, R. Woodrow Setzer

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Description of Tables S1 through S3. Tables S1, S2, and S3 provide information on NHANES 2009-2010 chemicals from Groups A, B, and C, respectively. From left to right, the columns in this table are:

- "NHANES Code", the label used by NHANES to identify the concentration of a given chemical measured in the urine or serum of subjects;
- "DSSTox RID", the source record identifier for the chemical in the DSSTox database (US Environmental Protection Agency 2016a);
- "DSSTox SID", the generic substance identifier for the chemical in the DSSTox database;
- "NHANES Chemical Name", the name given for the chemical in the NHANES 2009-2010 documentation;
- "CASN", a Chemical Abstract Service Registry Number corresponding to the chemical;
- "NHANES File", the name of the NHANES SAS transport (XPT) file that contains concentration information for the chemical; and
- "Proportion > Median", the estimated proportion of US residents (based on subject weights) in which the chemical concentration is greater than the median concentration.

One can find detailed information on any chemical listed in these tables by entering the relevant DSSTox SID into the CompTox Dashboard search engine (US Environmental Protection Agency 2016b).

Table S1. Listing of Group A chemicals from NHANES 2009-2010.

NHANES Code	DSSTox RID	DSSTox SID	NHANES Chemical Name	CASN	NHANES File	Proportion > Median
URXUSB	DTXRID802675623	DTXSID5023879	Antimony	7440-36-0	UHM_F	0.499841
URXUBA	DTXRID502675624	DTXSID8023894	Barium	7440-39-3	UHM_F	0.499944
URXUBE	DTXRID202675625	DTXSID4023913	Beryllium	7440-41-7	UHM_F	0
URXUCD	DTXRID902675626	DTXSID1023940	Cadmium	7440-43-9	UHM_F	0.499799
URXUCS	DTXRID602675627	DTXSID5036767	Cesium	7440-46-2	UHM_F	0.499647
URXUCO	DTXRID302675628	DTXSID1031040	Cobalt	7440-48-4	UHM_F	0.499281
URXUPB	DTXRID002675629	DTXSID2024161	Lead	7439-92-1	UHM_F	0.49821
URXUMO	DTXRID302675630	DTXSID1024207	Molybdenum	7439-98-7	UHM_F	0.499482
URXUPT	DTXRID002675631	DTXSID9064681	Platinum	7440-06-4	UHM_F	0.118602
URXUTL	DTXRID702675632	DTXSID2036035	Thallium	7440-28-0	UHM_F	0.499981
URXUTU	DTXRID402675633	DTXSID8052481	Tungsten	7440-33-7	UHM_F	0.499485
URXUUR	DTXRID102675634	DTXSID1042522	Uranium	7440-61-1	UHM_F	0.499603
URXUAS	DTXRID702675606	DTXSID4023886	Arsenic	7440-38-2	UAS_F	0.499925
URXUAS5	DTXRID402675607	DTXSID1034341	Arsenic (V) acid	7778-39-4	UAS_F	0.023311
URXUAB	DTXRID102675608	DTXSID0052833	Arsenobetaine	64436-13-1	UAS_F	0.499981
URXUAC	DTXRID802675609	DTXSID80873153	Arsenocholine	39895-81-3	UAS_F	0.022656
URXUAS3	DTXRID102675610	DTXSID7074828	Arsenous (III) acid	13464-58-9	UAS_F	0.044339
URXUDMA	DTXRID802675611	DTXSID7020508	Dimethylarsonic acid	75-60-5	UAS_F	0.499605
URXUMMA	DTXRID502675612	DTXSID4020903	Monomethylarsonic acid	124-58-3	UAS_F	0.305048
URXUTM	DTXRID202675613	DTXSID1021401	Trimethylarsine oxide	4964-14-1	UAS_F	0.006581
URXNO3	DTXRID902675614	DTXSID5024217	Nitrate	14797-55-8	PERNT_F	0.499838
URXUP8	DTXRID602675615	DTXSID6024252	Perchlorate	14797-73-0	PERNT_F	0.49903
URXSCN	DTXRID302675616	DTXSID8047763	Thiocyanate	302-04-5	PERNT_F	0.499518
URXDAZ	DTXRID002675617	DTXSID9022310	Daidzein	486-66-8	PHYTO_F	0.499496
URXETD	DTXRID702675618	DTXSID0047876	Enterodiol	80226-00-2	PHYTO_F	0.499773
URXETL	DTXRID402675619	DTXSID0048183	Enterolactone	78473-71-9	PHYTO_F	0.499854
URXEQU	DTXRID702675620	DTXSID7058705	Equol	94105-90-5	PHYTO_F	0.499887
URXGNS	DTXRID402675621	DTXSID5022308	Genistein	446-72-0	PHYTO_F	0.499779
URXDMA	DTXRID102675622	DTXSID40873154	O-Desmethylangolensin	21255-69-6	PHYTO_F	0.498984

Table S2. Listing of Group B chemicals from NHANES 2009-2010.

NHANES Code	DSSTox RID	DSSTox SID	NHANES Chemical Name	CASN	NHANES File	Proportion > Median
URXBP3	DTXRID802675635	DTXSID3022405	Benzophenone-3	131-57-7	EPH_F	0.499568
URXBPH	DTXRID502675636	DTXSID7020182	Bisphenol A	80-05-7	EPH_F	0.499183
URX4TO	DTXRID202675637	DTXSID9022360	4-tert-Octylphenol	140-66-9	EPH_F	0.111579
URXTRS	DTXRID902675638	DTXSID5032498	Triclosan	3380-34-5	EPH_F	0.499997
URXBUP	DTXRID602675639	DTXSID3020209	Butyl paraben	94-26-8	EPH_F	0.385113
URXEPB	DTXRID902675640	DTXSID9022528	Ethyl paraben	120-47-8	EPH_F	0.49988
URXMPB	DTXRID602675641	DTXSID4022529	Methyl paraben	99-76-3	EPH_F	0.499836
URXPPB	DTXRID302675642	DTXSID4022527	n-Propyl paraben	94-13-3	EPH_F	0.498906
URXOPP	DTXRID002675643	DTXSID2021151	ortho-Phenylphenol	90-43-7	PP_F	0.213037
URX1TB	DTXRID702675644	DTXSID4024359	2,4,5-Trichlorophenol	95-95-4	PP_F	0.248461
URX3TB	DTXRID402675645	DTXSID5021386	2,4,6-Trichlorophenol	88-06-2	PP_F	0.251625
URXDCB	DTXRID102675646	DTXSID1020439	2,4-Dichlorophenol	120-83-2	PP_F	0.499796
URX14D	DTXRID802675647	DTXSID7025003	2,5-Dichlorophenol	583-78-8	PP_F	0.499518
URXMZP	DTXRID502675648	DTXSID9043938	Mono-benzyl phthalate	2528-16-7	PHTHTE_F	0.499746
URXMIB	DTXRID202675649	DTXSID5052701	Mono-isobutyl phthalate	30833-53-5	PHTHTE_F	0.499786
URXMBP	DTXRID502675650	DTXSID4040002	Mono-n-butyl phthalate	131-70-4	PHTHTE_F	0.49988
URXMCP	DTXRID202675651	DTXSID3052729	Mono-cyclohexyl phthalate	7517-36-4	PHTHTE_F	0.044604
URXMEP	DTXRID902675652	DTXSID3052696	Mono-ethyl phthalate	2306-33-4	PHTHTE_F	0.499813
URXMHP	DTXRID602675653	DTXSID2025680	Mono-2-ethylhexyl phthalate	4376-20-9	PHTHTE_F	0.499816
URXMHH	DTXRID302675654	DTXSID50873160	Mono-(2-ethyl-5-hydroxyhexyl) phthalate	40321-99-1	PHTHTE_F	0.499549
URXMOH	DTXRID002675655	DTXSID00865994	Mono-(2-ethyl-5-oxohexyl) phthalate	40321-98-0	PHTHTE_F	0.499876
URXECP	DTXRID702675656	DTXSID20873152	Mono-(2-ethyl-5-carboxypentyl) phthalate	40809-41-4	PHTHTE_F	0.499757
URXCNP	DTXRID402675657	DTXSID60873156	Mono-(carboxynonyl) phthalate	1373125-93-9	PHTHTE_F	0.499901
URXMNP	DTXRID102675658	DTXSID20873157	Mono-isononyl phthalate	519056-28-1	PHTHTE_F	0.391561
URXCOP	DTXRID802675659	DTXSID00873155	Mono-(carboxyoctyl) phthalate	1923895-92-4	PHTHTE_F	0.499889
URXMNM	DTXRID102675660	DTXSID9040001	Mono-methyl phthalate	4376-18-5	PHTHTE_F	0.499155
URXMC1	DTXRID802675661	DTXSID8052726	Mono-(3-carboxypropyl) phthalate	66851-46-5	PHTHTE_F	0.499539
URXMOP	DTXRID502675662	DTXSID4052714	Mono-n-octyl phthalate	5393-19-1	PHTHTE_F	0.021904
URXP04	DTXRID202675663	DTXSID2047569	2-Hydroxyfluorene	2443-58-5	PAH_F	0.499159
URXP03	DTXRID902675664	DTXSID9047540	3-Hydroxyfluorene	6344-67-8	PAH_F	0.499818
URXP17	DTXRID602675665	DTXSID4052683	9-Hydroxyfluorene	1689-64-1	PAH_F	0.499253
URXP06	DTXRID302675666	DTXSID90872758	1-Hydroxyphenanthrene	2433-56-9	PAH_F	0.499683
URXP07	DTXRID002675667	DTXSID8052722	2-Hydroxyphenanthrene	605-55-0	PAH_F	0.499147
URXP05	DTXRID702675668	DTXSID3052723	3-Hydroxyphenanthrene	605-87-8	PAH_F	0.499623
URXP10	DTXRID402675669	DTXSID1038298	1-Hydroxypyrene	5315-79-7	PAH_F	0.499346
URXP01	DTXRID702675670	DTXSID6021793	1-Hydroxynapthalene	90-15-3	PAH_F	0.499626
URXP02	DTXRID402675671	DTXSID5027061	2-Hydroxynapthalene	135-19-3	PAH_F	0.499959

Table S3. Listing of Group C chemicals from NHANES 2009-2010.

NHANES Code	DSSTox RID	DSSTox SID	NHANES Chemical Name	CASN	NHANES File	Proportion > Median
URX24D	DTXRID402675702	DTXSID0020442	2,4-Dichlorophenoxyacetic acid	94-75-7	UPHOPM_F	0.499183
URX25T	DTXRID102675703	DTXSID5021388	2,4,5-Trichlorophenoxyacetic acid	93-76-5	UPHOPM_F	0.001142
URXMAL	DTXRID802675704	DTXSID7052739	Malathion dicarboxylic acid	1190-28-9	UPHOPM_F	0.170047
URXOXY	DTXRID502675705	DTXSID1027502	2-Isopropyl-4-methyl-6-hydroxypyrimidine	2814-20-2	UPHOPM_F	0.12162
URXPAR	DTXRID202675706	DTXSID0021834	para-Nitrophenol	100-02-7	UPHOPM_F	0.499841
URXCPM	DTXRID902675707	DTXSID7038317	3,5,6-Trichloro-2-pyridinol	6515-38-4	UPHOPM_F	0.499782
URXTCC	DTXRID602675708	DTXSID9052717	trans-3-(2,2-Dichlorovinyl)-2,2-dimethylcyclopropane carboxylic acid	55701-03-6	UPHOPM_F	0.115931
URXCB3	DTXRID302675709	DTXSID40873159	cis-3-(2,2-Dibromovinyl)-2,2-dimethylcyclopropane carboxylic acid	53179-78-5	UPHOPM_F	0.012149
URX4FP	DTXRID602675710	DTXSID00228005	4-Fluoro-3-phenoxybenzoic acid	77279-89-1	UPHOPM_F	0.042239
URXOPM	DTXRID302675711	DTXSID1038321	3-Phenoxybenzoic acid	3739-38-6	UPHOPM_F	0.499127
LBXPFBS	DTXRID902675690	DTXSID5030030	Perfluorobutane sulfonic acid	375-73-5	PFC_F	0.008512
LBXPFDE	DTXRID602675691	DTXSID3031860	Perfluorodecanoic acid	335-76-2	PFC_F	0.342616
LBXPFDO	DTXRID302675692	DTXSID8031861	Perfluorododecanoic acid	307-55-1	PFC_F	0.048056
LBXPFHP	DTXRID002675693	DTXSID1037303	Perfluoroheptanoic acid	375-85-9	PFC_F	0.205618
LBXPFHS	DTXRID702675694	DTXSID7040150	Perfluorohexane sulfonic acid	355-46-4	PFC_F	0.4889
LBXPFNA	DTXRID402675695	DTXSID8031863	Perfluorononanoic acid	375-95-1	PFC_F	0.467424
LBXPFOA	DTXRID102675696	DTXSID8031865	Perfluorooctanoic acid	335-67-1	PFC_F	0.485585
LBXPFOS	DTXRID802675697	DTXSID3031864	Perfluorooctane sulfonic acid	1763-23-1	PFC_F	0.499721
LBXPFSA	DTXRID502675698	DTXSID3038939	Perfluorooctane sulfonamide	754-91-6	PFC_F	0.000615
LBXEPAH	DTXRID202675699	DTXSID5062760	2-(N-Ethyl-perfluorooctane sulfonamido) acetic acid	2991-50-6	PFC_F	0.052624
LBXMPAH	DTXRID002675700	DTXSID10624392	2-(N-Methyl-perfluorooctane sulfonamido) acetic acid	2355-31-9	PFC_F	0.420071
LBXPFUA	DTXRID702675701	DTXSID8047553	Perfluoroundecanoic acid	2058-94-8	PFC_F	0.306954
URXMU1	DTXRID102675672	DTXSID70221063	1-Methyluric acid	708-79-2	CAFE_F	0.499746
URXMU2	DTXRID802675673	DTXSID50209243	3-Methyluric acid	605-99-2	CAFE_F	0.499944
URXMU3	DTXRID502675674	DTXSID40210106	7-Methyluric acid	612-37-3	CAFE_F	0.499673
URXMU4	DTXRID202675675	DTXSID50241466	1,3-Dimethyluric acid	944-73-0	CAFE_F	0.499226
URXMU5	DTXRID902675676	DTXSID30187499	1,7-Dimethyluric acid	33868-03-0	CAFE_F	0.499427
URXMU6	DTXRID602675677	DTXSID10156769	3,7-Dimethyluric acid	13087-49-5	CAFE_F	0.499352
URXMU7	DTXRID302675678	DTXSID50202496	1,3,7-Trimethyluric acid	5415-44-1	CAFE_F	0.499264

URXMX1	DTXRID002675679	DTXSID30210271	1-Methylxanthine	6136-37-4	CAFE_F	0.499538
URXMX2	DTXRID302675680	DTXSID90148107	3-Methylxanthine	1076-22-8	CAFE_F	0.499002
URXMX3	DTXRID002675681	DTXSID60203696	7-Methylxanthine	552-62-5	CAFE_F	0.499956
URXMX4	DTXRID702675682	DTXSID5021336	1,3-Dimethylxanthine	58-55-9	CAFE_F	0.499835
URXMX5	DTXRID402675683	DTXSID2052281	1,7-Dimethylxanthine	611-59-6	CAFE_F	0.499834
URXMX6	DTXRID102675684	DTXSID9026132	3,7-Dimethylxanthine	83-67-0	CAFE_F	0.499745
URXMX7	DTXRID802675685	DTXSID0020232	1,3,7-Trimethylxanthine	58-08-2	CAFE_F	0.49957
URXAMU	DTXRID502675686	DTXSID20173669	AAMU	19893-78-8	CAFE_F	0.499327
URXDEE	DTXRID202675687	DTXSID2021995	N,N-diethyl-meta-toluamide	134-62-3	DEET_F	0.033173
URXDEA	DTXRID902675688	DTXSID30222551	3-diethyl-carbamoyl benzoic acid	72236-23-8	DEET_F	0.499823
URXDHD	DTXRID602675689	DTXSID70222550	N,N-diethyl-3-hydroxymethylbenzamide	72236-22-7	DEET_F	0.170411

Description of Tables S4 through S6. Tables S4, S5, and S6 provide information about concordance percentages obtained between sets of prevalent combinations obtained using the entire subsample A, B, or C, respectively, from NHANES 2009-2010 or partitions the subsample. Row names indicate the first set of prevalent combinations (c_i) considered in computing the concordance percentage. For example, "A/30%" indicates the set of prevalent combinations obtained when applying FIM to all of subsample A using a minimum prevalence level of 30% and "A:P2/30%" indicates the set of prevalent combinations obtained when applying FIM to just the second partition of subsample A using a minimum prevalence level of 30%. Column names indicate the second set of prevalent combination (c_j) considered in computing the concordance percentage. These are named using the same convention.

Table S4. Listing of concordance percentages between sets of prevalent combinations obtained using the entire subsample A from NHANES 2009-2010 or partitions thereof.

	A/30%	A:P1/30%	A:P2/30%	A:P3/30%	A:P4/30%	A/28%	A:P1/28%	A:P2/28%	A:P3/28%	A:P4/28%
A/30%	1.000	0.903	0.839	0.742	0.903	1.000	1.000	1.000	0.968	1.000
A:P1/30%	0.903	1.000	0.839	0.710	0.839	1.000	1.000	1.000	0.935	0.968
A:P2/30%	0.722	0.722	1.000	0.639	0.667	1.000	0.889	1.000	0.861	0.972
A:P3/30%	0.767	0.733	0.767	1.000	0.767	0.933	0.833	0.933	1.000	0.933
A:P4/30%	0.757	0.703	0.649	0.622	1.000	1.000	0.892	0.919	0.865	1.000

Table S5. Listing of concordance percentages between sets of prevalent combinations obtained using the entire subsample B from NHANES 2009-2010 or partitions thereof.

	B/33%	B:P1/33%	B:P2/33%	B:P3/33%	B:P4/33%	B/31%	B:P1/31%	B:P2/31%	B:P3/31%	B:P4/31%
B/33%	1.000	0.933	0.883	0.967	0.950	1.000	1.000	0.983	1.000	1.000
B:P1/33%	0.949	1.000	0.847	0.949	0.949	1.000	1.000	0.983	1.000	1.000
B:P2/33%	0.869	0.820	1.000	0.836	0.852	1.000	0.934	1.000	0.951	0.951
B:P3/33%	0.921	0.889	0.810	1.000	0.905	1.000	1.000	0.968	1.000	0.984
B:P4/33%	0.934	0.918	0.852	0.934	1.000	0.984	0.984	0.984	0.984	1.000

Table S6. Listing of concordance percentages between sets of prevalent combinations obtained using the entire subsample C from NHANES 2009-2010 or partitions thereof.

	C/40%	C:P1/40%	C:P2/40%	C:P3/40%	C:P4/40%	C/38%	C:P1/38%	C:P2/38%	C:P3/38%	C:P4/38%
C/40%	1.000	0.806	0.935	0.855	0.855	1.000	1.000	1.000	0.984	1.000
C:P1/40%	0.926	1.000	0.889	0.907	0.833	1.000	1.000	0.963	0.981	0.981
C:P2/40%	0.866	0.716	1.000	0.746	0.806	0.970	0.955	1.000	0.940	0.985
C:P3/40%	0.964	0.891	0.909	1.000	0.873	1.000	1.000	1.000	1.000	1.000
C:P4/40%	0.898	0.763	0.915	0.814	1.000	0.983	0.966	1.000	0.949	1.000

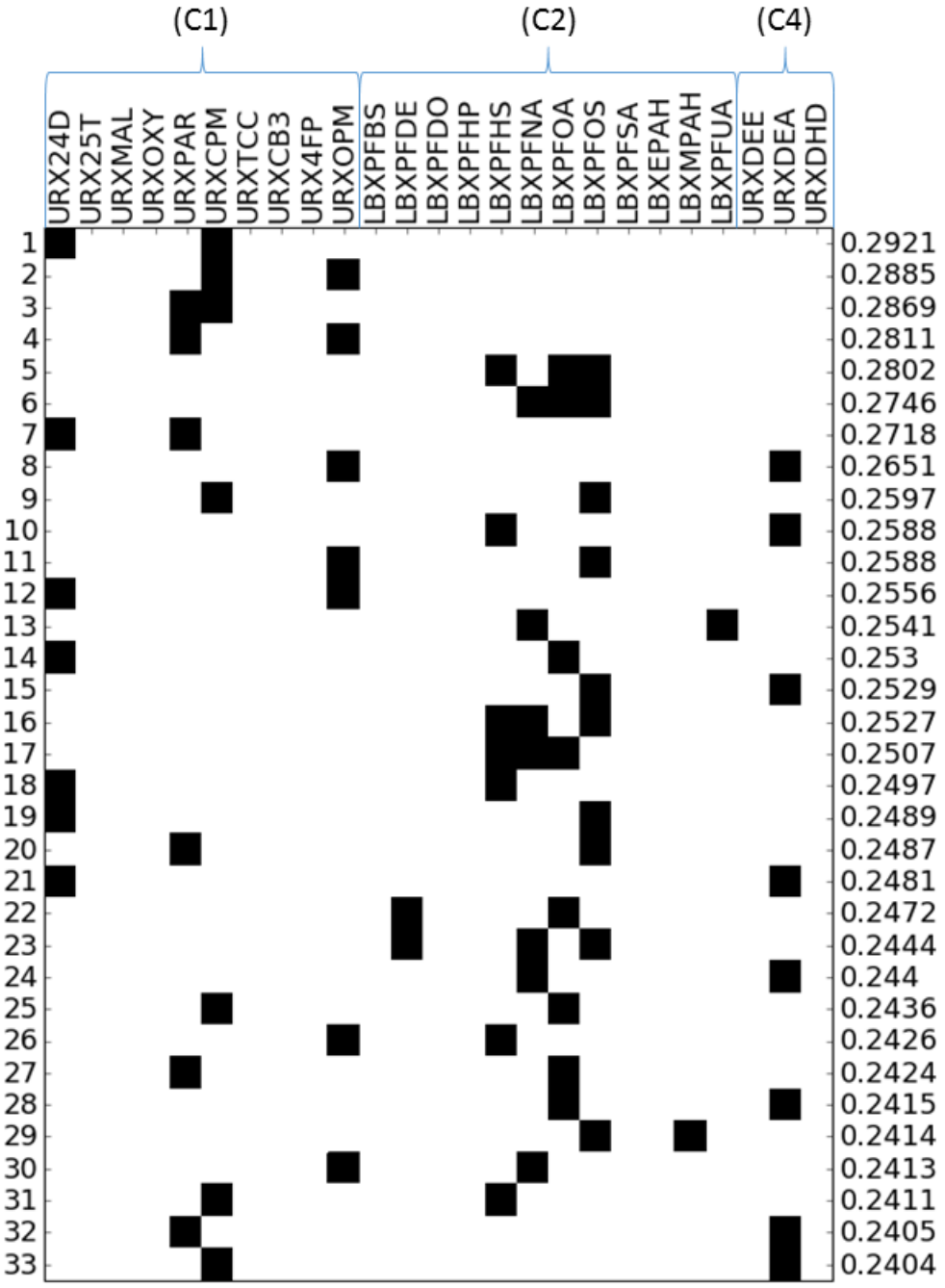

Figure S1. Presence-absence map (black indicates present) illustrating 33 maximal prevalent combinations of Group C chemicals from subgroups C1, C2, and C4 (cf. Section 2.1.1 of manuscript). The maximal prevalent combinations were identified by omitting Subgroup C3 chemicals from consideration and then applying FIM with discretization thresholds set at the 50th percentiles and a minimum prevalence level of 24%. NHANES codes along the top of the figure indicate Group C chemicals, and these are organized into subgroups C1, C2, and C4. (Note that subgroup C3 has been omitted.) The observed prevalence number at the right of each row indicates the proportion of US residents in which the given combination was observed to occur.

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