

Supplemental Figures and Tables for:

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WellExplorer: An Integrative Resource Linking Hydraulic Fracturing Chemicals with Hormonal Pathways and Geographic Location

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SUPPLEMENTAL MATERIAL**Table S1. Hydraulic Fracturing Ingredients Targeting Estrogen, Testosterone or Hormone Pathways**

CAS Number	Chemical Name
Chemicals Targeting Estrogen Pathways	
101-77-9	Benzenamine, 4,4'-methylenebis-
104-40-5	Nonyl Phenol, 4 Mol
106-24-1	2,6-Octadien-1-ol, 3,7-dimethyl-, (2E)-
107-02-8	Acrolein
107-98-2	1-Methoxy-2-Propanol
108-38-3	Benzene, 1,3-dimethyl-(Xylene)
108-83-8	Disobutyl Ketone
110-17-8	Fumaric Acid
111-42-2	Diethanolamine
111-44-4	Dichloroethyl ether (DCEE)
117-81-7	Di (2ethylhexyl) Phthalate
126-92-1	Sodium-2-ethylhexyl sulfate
1344-28-1	Aluminum Oxide
138-22-7	Butyl lactate
139-13-9	Nitriloacetic Acid
151-21-3	Lauryl Sulfate
1762-95-4	Ammonium Thiocyanate
25322-69-4	Polypropylene Glycol
486-66-8	Soy Isoflavone
50-28-2	Silica Substrate
52-51-7	2-Bromo-2-Nitro-1,3-Propanediol
62-56-6	Thiourea
65-85-0	Benzoic Acid
7429-90-5	Aluminum Needles
7440-02-0	Nickel
7446-70-0	Aluminum Chloride
7646-79-9	Cobalt chloride(CoCl ₂)
7664-38-2	Phosphoric Acid
7718-54-9	Nickel(II) Chloride
7786-81-4	Nickel Sulfate
78-40-0	Triethyl Phosphate
872-50-4	N-Methyl Pyrrolidone
9004-82-4	Alpha-Sulfo-w-(dodecyloxy)-poly(oxyethane-1,2-diyl), sodium salt
92-52-4	BIPHENYL
Chemicals Targeting Testosterone Pathways	
10025-91-9	Antimony trichloride
107-98-2	1-Methoxy-2-Propanol
111-30-8	Glutaraldehyde
111-40-0	Diethylenetriamine
25038-59-9	Polyethyleneterephthalate
50-28-2	Silica Substrate
533-74-4	3,5-Dimethyltetrahydro-1,3,5-thiadiazine-2-thione
8001-54-5	Quaternary ammonium compounds, alkylbenzyltrimethyl, chlorides
Chemicals Targeting Hormone Pathways	
10025-91-9	Antimony trichloride
101-77-9	Benzenamine, 4,4'-methylenebis-
104-40-5	Nonyl Phenol, 4 Mol
106-24-1	2,6-Octadien-1-ol, 3,7-dimethyl-,(2E)-

107-98-2	1-Methoxy-2-Propanol
108-38-3	Benzene, 1,3-dimethyl-(Xylene)
108-83-8	Diisobutyl Ketone
111-30-8	Glutaraldehyde
111-40-0	Diethylenetriamine
111-42-2	Diethanolamine
111-44-4	Dichloroethyl ether (DCEE)
112-80-1	Oleic Acid
117-81-7	Di (2ethylhexyl) Phthalate
1184-78-7	Trimethylamine, N-oxide
126-92-1	Sodium-2-ethylhexyl sulfate
128-37-0	Butylated hydroxytoluene
1344-28-1	Aluminum Oxide
138-22-7	Butyl lactate
139-13-9	Nitriloacetic Acid
151-21-3	Lauryl Sulfate
1762-95-4	Ammonium Thiocyanate
25038-59-9	Polyethyleneterephthalate
2634-33-5	1,2-Benzisothiazolin-3-one
486-66-8	Soy Isoflavone
50-28-2	Silica Substrate
52-51-7	2-Bromo-2-nitro-1,3-propanediol
533-74-4	3,5-Dimethyltetrahydro-1,3,5-thiadiazine-2-thione
56-86-0	L-Glutamic acid
62-56-6	Thiourea
64-17-5	Ethyl Alcohol
64-19-7	Acetic Acid
65-85-0	Benzoic Acid
71-43-2	Benzene
71-48-7	Cobalt Acetate
7429-90-5	Aluminum Needles
7440-02-0	Nickel
7446-70-0	Aluminium Chloride
7487-88-9	Magnesium Sulfate
75-50-3	Trimethylamine
7646-79-9	Cobalt chloride(CoCl ₂)
7664-38-2	Phosphoric Acid
7664-41-7	Ammonia
7718-54-9	Nickel(II) Chloride
7772-99-8	Stannous Chloride Dihydrate
7786-81-4	Nickel Sulfate
78-40-0	Triethyl Phosphate
80-08-0	4,4'-Diaminodiphenyl sulfone
8001-54-5	Quaternary ammonium compounds, alkylbenzyltrimethyl, chlorides
9004-82-4	Alpha-Sulfo-w-(dodecyloxy)-poly(oxyethane-1,2-diyl), sodium salt
91-20-3	Naphthalene
92-52-4	BIPHENYL

Gene Name	Full Gene Name	Specific Function	Gene Synonyms	KEGG ID	Estrogen Gene	Hormone Gene	Testosterone Gene
ESR1	Estrogen receptor	Nuclear hormone receptor...	ER; ER-alpha; ESR; Estradiol receptor; NR3A1; Nuclear receptor subfamily 3 group A member 1	hsa:2099	Yes	Yes	No
HSD17B1	Estradiol 17-beta-dehydrogenase 1	Favors the reduction of estrogens and androgens...	1.1.1.62; 17-beta-HSD 1; 17-beta-hydroxysteroid dehydrogenase type 1...	hsa:3292	Yes	No	No
HSD3B1	3 beta-hydroxysteroid dehydrogenase/Delta 5-->4-isomerase type 1	3-beta-HSD is a bifunctional enzyme... dihydrotestosterone to 5-alpha-androstane-3 beta,17 beta-diol...	3 beta-hydroxysteroid dehydrogenase/Delta 5-->4-isomerase type I; 3-beta-HSD I; 3BH; HSDB3A; Trophoblast antigen FDO161	hsa:3283	No	No	Yes
JAK2	Tyrosine-protein kinase JAK2	...plays a pivotal role in signal transduction via its association with type I receptors such as growth hormone (GHR), prolactin (PRLR)...	2.7.10.2; JAK-2; Janus kinase 2	hsa:3717	No	Yes	No

KEGG ID Used to Identify
Other Genes in Same
Pathway

Figure S1. Illustrative Diagram Detailing the Method of Linking Genes to Estrogen, Hormone and Testosterone Genes and Pathways. The pathway linkage was done using the KEGG IDs. For example, JAK2 is labeled as a hormone gene with corresponding KEGG ID (hsa:3717) any other genes in T3DB containing the same KEGG ID (hsa:3717) would be labeled as belonging to the hormone pathway even if the word 'hormone' was not explicitly found in the name, specific function or synonym fields.