

Appendix A. Proof-of-Concept (POC) Subset of the Non-confidential TSCA Active Inventory

CASRN	DTXSID	PREFERRED_NAME
156-60-5	DTXSID7024031	(E)-1,2-Dichloroethylene
79-33-4	DTXSID6034689	(S)-2-Hydroxypropionic acid
54464-59-4	DTXSID5052200	1-(1,2,3,4,5,6,7,8-Octahydro-2,3,5,5-tetramethyl-2-naphthyl)ethan-1-one
68155-66-8	DTXSID9052397	1-(1,2,3,5,6,7,8,8a-Octahydro-2,3,8,8-tetramethyl-2-naphthyl)ethan-1-one
68155-67-9	DTXSID6041923	1-(2,3,8,8-Tetramethyl-1,2,3,4,6,7,8,8a-octahydronaphthalen-2-yl)ethanone
79-34-5	DTXSID7021318	1,1,2,2-Tetrachloroethane
79-00-5	DTXSID5021380	1,1,2-Trichloroethane
75-34-3	DTXSID1020437	1,1-Dichloroethane
1163-19-5	DTXSID9020376	1,1'-Oxybis[2,3,4,5,6-pentabromobenzene]
110-98-5	DTXSID7026863	1,1'-Oxybis-2-propanol
96-18-4	DTXSID9021390	1,2,3-Trichloropropane
120-82-1	DTXSID0021965	1,2,4-Trichlorobenzene
3194-55-6	DTXSID4027527	1,2,5,6,9,10-Hexabromocyclododecane
106-93-4	DTXSID3020415	1,2-Dibromoethane
95-50-1	DTXSID6020430	1,2-Dichlorobenzene
107-06-2	DTXSID6020438	1,2-Dichloroethane
78-87-5	DTXSID0020448	1,2-Dichloropropane
6920-22-5	DTXSID40863959	1,2-Hexanediol
57-55-6	DTXSID0021206	1,2-Propylene glycol
106-99-0	DTXSID3020203	1,3-Butadiene
99-65-0	DTXSID9024065	1,3-Dinitrobenzene
102-06-7	DTXSID3025178	1,3-Diphenylguanidine

106-46-7	DTXSID1020431	1,4-Dichlorobenzene
123-91-1	DTXSID4020533	1,4-Dioxane
106-94-5	DTXSID6021874	1-Bromopropane
71-36-3	DTXSID1021740	1-Butanol
88-73-3	DTXSID0020280	1-Chloro-2-nitrobenzene
100-00-5	DTXSID5020281	1-Chloro-4-nitrobenzene
661-19-8	DTXSID4027286	1-Docosanol
629-96-9	DTXSID0027272	1-Eicosanol
36653-82-4	DTXSID4027991	1-Hexadecanol
112-92-5	DTXSID8026935	1-Octadecanol
111-87-5	DTXSID7021940	1-Octanol
118-96-7	DTXSID7024372	2,4,6-Trinitrotoluene
732-26-3	DTXSID2021311	2,4,6-Tris(tert-butyl)phenol
51-28-5	DTXSID0020523	2,4-Dinitrophenol
121-14-2	DTXSID0020529	2,4-Dinitrotoluene
108-31-6	DTXSID7024166	2,5-Furandione
96-29-7	DTXSID1021821	2-Butanone oxime
110-44-1	DTXSID3021277	2E,4E-Hexadienoic acid
183658-27-7	DTXSID9052686	2-Ethylhexyl 2,3,4,5-tetrabromobenzoate
149-30-4	DTXSID1020807	2-Mercaptobenzothiazole
109-86-4	DTXSID5024182	2-Methoxyethanol
78-83-1	DTXSID0021759	2-Methyl-1-propanol
534-52-1	DTXSID1022053	2-Methyl-4,6-dinitrophenol
55583-69-2	DTXSID70873187	2-Methylallyl alcohol ethoxylate
88-74-4	DTXSID1025726	2-Nitroaniline
79-94-7	DTXSID1026081	3,3',5,5'-Tetrabromobisphenol A
91-94-1	DTXSID6020432	3,3'-Dichlorobenzidine

612-83-9	DTXSID1020433	3,3'-Dichlorobenzidine dihydrochloride
591-35-5	DTXSID2025006	3,5-Dichlorophenol
4435-53-4	DTXSID2052106	3-Methoxybutyl acetate
99-08-1	DTXSID5021831	3-Nitrotoluene
140-66-9	DTXSID9022360	4-(1,1,3,3-Tetramethylbutyl)phenol
17540-75-9	DTXSID8029315	4-(Butan-2-yl)-2,6-di-tert-butylphenol
16090-02-1	DTXSID0027777	4,4'-Bis(2-morpholino-4-anilino-s-triazinyl-6-amino)stilbene-2,2'-disulfonic acid disodium salt
101-14-4	DTXSID5020865	4,4'-Methylenebis(2-chloroaniline)
80-51-3	DTXSID7026499	4,4'-Oxybis(benzenesulfohydrazide)
101-80-4	DTXSID0021094	4,4'-Oxydianiline
136-85-6	DTXSID1038743	5-Methyl-1H-benzotriazole
51-52-5	DTXSID5021209	6-Propyl-2-thiouracil
75-07-0	DTXSID5039224	Acetaldehyde
103-90-2	DTXSID2020006	Acetaminophen
79-06-1	DTXSID5020027	Acrylamide
79-10-7	DTXSID0039229	Acrylic acid
107-13-1	DTXSID5020029	Acrylonitrile
3825-26-1	DTXSID8037708	Ammonium perfluorooctanoate
62-53-3	DTXSID8020090	Aniline
NOCAS_8724 14	DTXSID30872414	Antimony & Antimony Compounds
NOCAS_8724 15	DTXSID90872415	Arsenic & Arsenic Compounds
137-66-6	DTXSID3041611	Ascorbyl palmitate
50-78-2	DTXSID5020108	Aspirin
1912-24-9	DTXSID9020112	Atrazine
25057-89-0	DTXSID0023901	Bentazone

1302-78-9	DTXSID6030782	Bentonite
71-43-2	DTXSID3039242	Benzene
65-85-0	DTXSID6020143	Benzoic acid
119-61-9	DTXSID0021961	Benzophenone
85-68-7	DTXSID3020205	Benzyl butyl phthalate
26040-51-7	DTXSID7027887	Bis(2-ethylhexyl) tetrabromophthalate
103-23-1	DTXSID0020606	Bis(2-ethylhexyl)hexanedioate
80-05-7	DTXSID7020182	Bisphenol A
75-25-2	DTXSID1021374	Bromoform
128-37-0	DTXSID2020216	Butylated hydroxytoluene
17852-99-2	DTXSID2066270	C.I. Pigment Red 52, calcium salt (1:1)
5567-15-7	DTXSID1021453	C.I. Pigment Yellow 83
7440-43-9	DTXSID1023940	Cadmium
NOCAS_8724 17	DTXSID10872417	Cadmium & Cadmium Compounds
58-08-2	DTXSID0020232	Caffeine
62-54-4	DTXSID0020234	Calcium acetate
299-28-5	DTXSID2029618	Calcium D-gluconate
105-60-2	DTXSID4020240	Caprolactam
10605-21-7	DTXSID4024729	Carbendazim
56-23-5	DTXSID8020250	Carbon tetrachloride
513-77-9	DTXSID1029623	Carbonic acid, barium salt (1:1)
1698-60-8	DTXSID3034872	Chloridazon
108-90-7	DTXSID4020298	Chlorobenzene
143-28-2	DTXSID0022010	cis-Oleyl alcohol
77-92-9	DTXSID3020332	Citric acid
1702-17-6	DTXSID9029221	Clopyralid

NOCAS_8724 19	DTXSID30872419	Cobalt & Cobalt Compounds
7646-79-9	DTXSID9040180	Cobalt chloride
64-86-8	DTXSID5024845	Colchicine
8001-58-9	DTXSID2023987	Creosote
420-04-2	DTXSID9034490	Cyanamide
NOCAS_8724 20	DTXSID40872420	Cyanide salts
1222-05-5	DTXSID8027373	Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl-
134-62-3	DTXSID2021995	DEET
50-02-2	DTXSID3020384	Dexamethasone
81-13-0	DTXSID3022906	Dexpanthenol
50-70-4	DTXSID5023588	D-Glucitol
526-95-4	DTXSID8027169	D-Gluconic acid
50-99-7	DTXSID7022910	D-Glucose
117-81-7	DTXSID5020607	Di(2-ethylhexyl) phthalate
131-17-9	DTXSID7020392	Diallyl phthalate
109-43-3	DTXSID1041847	Dibutyl decanedioate
84-74-2	DTXSID2021781	Dibutyl phthalate
75-09-2	DTXSID0020868	Dichloromethane
62-73-7	DTXSID5020449	Dichlorvos
99-30-9	DTXSID2020426	Dicloran
84-61-7	DTXSID5025021	Dicyclohexyl phthalate
105-53-3	DTXSID7021863	Diethyl propanedioate
111-77-3	DTXSID3025049	Diethylene glycol monomethyl ether
35367-38-5	DTXSID1024049	Diflubenzuron
84-69-5	DTXSID9022522	Diisobutyl phthalate

26761-40-0	DTXSID4025082	Diisodecyl phthalate
28553-12-0	DTXSID4022521	Diisononyl phthalate
60-51-5	DTXSID7020479	Dimethoate
108-59-8	DTXSID4029145	Dimethyl malonate
108-01-0	DTXSID2020505	Dimethylaminoethanol
117-84-0	DTXSID1021956	Di-n-octyl phthalate
25265-71-8	DTXSID0027856	Dipropylene glycol
88917-22-0	DTXSID4029062	Dipropylene glycol methyl ether acetate
330-54-1	DTXSID0020446	Diuron
69-65-8	DTXSID1023235	D-Mannitol
112-85-6	DTXSID3026930	Docosanoic acid
577-11-7	DTXSID8022959	Docusate sodium
9004-32-4	DTXSID2020555	Edifas B
759-94-4	DTXSID1024091	EPTC
64-17-5	DTXSID9020584	Ethanol
91-53-2	DTXSID9020582	Ethoxyquin
141-78-6	DTXSID1022001	Ethyl acetate
100-41-4	DTXSID3020596	Ethylbenzene
107-21-1	DTXSID8020597	Ethylene glycol
110-71-4	DTXSID0025286	Ethylene glycol dimethyl ether
75-21-8	DTXSID0020600	Ethylene oxide
60168-88-9	DTXSID2032390	Fenarimol
50-00-0	DTXSID7020637	Formaldehyde
446-72-0	DTXSID5022308	Genistein
106-24-1	DTXSID8026727	Geraniol
90-80-2	DTXSID0026549	Gluconolactone
111-30-8	DTXSID6025355	Glutaraldehyde

25637-99-4	DTXSID8025383	Hexabromocyclododecane
87-68-3	DTXSID7020683	Hexachloro-1,3-butadiene
118-74-1	DTXSID2020682	Hexachlorobenzene
51235-04-2	DTXSID4024145	Hexazinone
123-31-9	DTXSID7020716	Hydroquinone
54464-57-2	DTXSID7031290	Isocyclemone E
97-54-1	DTXSID7022413	Isoeugenol
78-79-5	DTXSID2020761	Isoprene
1332-58-7	DTXSID6049640	Kaolin
50-21-5	DTXSID7023192	Lactic acid
63-42-3	DTXSID2023193	Lactose
52-90-4	DTXSID8022876	L-Cysteine
NOCAS_8724 21	DTXSID00872421	Lead & Lead Compounds
63-68-3	DTXSID5040548	L-Methionine
NOCAS_8724 22	DTXSID60872422	Long-chain chlorinated paraffins (C18-20)
6915-15-7	DTXSID0027640	Malic acid
NOCAS_8724 23	DTXSID20872423	Medium-chain chlorinated paraffins (C14-17)
7487-94-7	DTXSID5020811	Mercuric chloride
67-56-1	DTXSID2021731	Methanol
625-45-6	DTXSID1031591	Methoxyacetic acid
74-83-9	DTXSID8020832	Methyl bromide
9004-67-5	DTXSID1036919	Methyl cellulose
99-76-3	DTXSID4022529	Methylparaben
NOCAS_8724 24	DTXSID80872424	Molybdenum & Molybdenum Compounds
31138-65-5	DTXSID7027966	Monosodium D-glucoheptonate

108-38-3	DTXSID6026298	m-Xylene
99-97-8	DTXSID0021832	N,N,4-Trimethylaniline
91-20-3	DTXSID8020913	Naphthalene
NOCAS_8724 25	DTXSID40872425	Nickel & Nickel Compounds
872-50-4	DTXSID6020856	N-Methyl-2-pyrrolidone
86-30-6	DTXSID6021030	N-Nitrosodiphenylamine
25154-52-3	DTXSID3021857	n-Nonylphenol
95-48-7	DTXSID8021808	o-Cresol
1843-05-6	DTXSID9027441	Octabenzene
556-67-2	DTXSID7027205	Octamethylcyclotetrasiloxane
124-07-2	DTXSID3021645	Octanoic acid
112-80-1	DTXSID1025809	Oleic acid
95-47-6	DTXSID3021807	o-Xylene
133-49-3	DTXSID3044540	Pentachlorobenzenethiol
87-86-5	DTXSID7021106	Pentachlorophenol
3296-90-0	DTXSID9020164	Pentaerythritol dibromide
375-73-5	DTXSID5030030	Perfluorobutanesulfonic acid
335-76-2	DTXSID3031860	Perfluorodecanoic acid
335-67-1	DTXSID8031865	Perfluorooctanoic acid
108-95-2	DTXSID5021124	Phenol
85-44-9	DTXSID2021159	Phthalic anhydride
1918-02-1	DTXSID1021160	Picloram
81-33-4	DTXSID9052555	Pigment Violet 29
6528-34-3	DTXSID0052336	Pigment Yellow 65
298-14-6	DTXSID0021177	Potassium bicarbonate
299-27-4	DTXSID7029617	Potassium D-gluconate
29420-49-3	DTXSID3037707	Potassium perfluorobutanesulfonate

106-42-3	DTXSID2021868	p-Xylene
108-46-3	DTXSID2021238	Resorcinol
68-26-8	DTXSID3023556	Retinol
127-47-9	DTXSID6021240	Retinol acetate
90-02-8	DTXSID1021792	Salicylaldehyde
122-34-9	DTXSID4021268	Simazine
497-19-8	DTXSID1029621	Sodium carbonate
4418-26-2	DTXSID7026029	Sodium dehydroacetate
527-07-1	DTXSID7027170	Sodium D-gluconate
7632-00-0	DTXSID0020941	Sodium nitrite
1344-09-8	DTXSID9029647	Sodium silicate
10102-17-7	DTXSID6044197	Sodium thiosulfate, pentahydrate
111-01-3	DTXSID0046513	Squalane
100-42-5	DTXSID2021284	Styrene
57-50-1	DTXSID2021288	Sucrose
994-05-8	DTXSID8024521	tert-Amyl methyl ether
127-18-4	DTXSID2021319	Tetrachloroethylene
58-55-9	DTXSID5021336	Theophylline
62-55-5	DTXSID9021340	Thioacetamide
137-26-8	DTXSID5021332	Thiram
7772-99-8	DTXSID8021351	Tin(II) chloride
126-73-8	DTXSID3021986	Tributyl phosphate
1461-22-9	DTXSID3027403	Tributyltin chloride
79-01-6	DTXSID0021383	Trichloroethylene
101-20-2	DTXSID4026214	Triclocarban
55335-06-3	DTXSID0032497	Triclopyr
77-93-0	DTXSID0040701	Triethyl citrate

2451-62-9	DTXSID4026262	Triglycidyl isocyanurate
115-86-6	DTXSID1021952	Triphenyl phosphate
68937-41-7	DTXSID4028880	Triphenyl phosphates isopropylated
24800-44-0	DTXSID7027837	Tripropylene glycol
55934-93-5	DTXSID8042503	Tripropylene glycol butyl ether
115-96-8	DTXSID5021411	Tris(2-chloroethyl) phosphate
75-01-4	DTXSID8021434	Vinyl chloride