

Appendix 7.1

Chemistry Specifications for Chemistry Services Contractors

National Toxicology Program

Examples of HTS Plate Maps and Structure Files

September 12, 2013

## Appendix 7.1 Examples of HTS Plate Maps and Structure Files.

### 1. Plate Map

1. A partial plate map is shown in Figure 1.

Figure 1.

	B	C	D	E	F	G	H	I	J	K	L	M	N
	Chemical Name	NTP SID	CHEM Task No	CAS Number	Lot No	Molecular Wt (g/mol)	Molecular Formula	Purity (%)	Final Conc (mM)	Aliquot volume (uL)	Supplier	Plate ID	Plate Position
2	Bisphenol A	557	CHEM10042	80-05-7	TX011629	228.2863	C15H16O2	99.7	20.3	80 Sigma	MRI00079	A03	
3	1-Naphthylamine	87	CHEM10042	134-32-7	1420454	143.1852	C10H9N	98	20.1	80 Sigma-Aldrich	MRI00079	A04	
4	Benomyl	511	CHEM10042	17804-35-2	08714PB	290.3177	C14H18N4O3	~ 95	19.9	80 Sigma-Aldrich	MRI00079	A05	
5	Dimethyl glutarate	741	CHEM10042	1119-40-0	358841/1	160.1678	C7H12O4	99.56	19.9	80 Fluka	MRI00079	A06	
6	Dazomet	683	CHEM10042	533-74-4	0203X	162.2763	C5H10N2S2	98.92	19.9	80 Sigma	MRI00079	A07	
7	Azathioprine	503	CHEM10042	446-86-6	TX005739	277.2626	C9H7N7O2S	98.4	19.9	80 Sigma	MRI00079	A08	
8	Butyl(2,4-dichlorophenoxy) acetate	159	CHEM10042	94-80-4	2267X	277.1438	C12H14Cl2O3	99.04	20.2	80 Sigma	MRI00079	A09	
9	m-Nitrobenzoic acid	979	CHEM10042	121-92-6	0330AH	167.1189	C7H5NO4	100	19.9	80 Unknown	MRI00079	A10	
10	Salicylazosulfapyridine	1266	CHEM10042	599-79-1	035K0968	398.3926	C18H14N4O5S	97.56	20.1	80 Sigma	MRI00079	A11	
11	benzylacetone	541	CHEM10042	2550-26-7	09111EH	148.2017	C10H12O	100	20.3	80 Sigma	MRI00079	A12	
12	1-Naphthalene acetic acid	86	CHEM10042	86-87-3	TX002225	186.2066	C12H10O2	99	20	80 ENAMINE	MRI00079	A13	
13	p-n-Nonylphenol	1136	CHEM10042	104-40-5	L867691	220.3505	C15H24O	100	20.2	80 Sigma	MRI00079	A14	
14	Butanal, 2-methyl-	2346	CHEM10042	96-17-3	013068J	86.1323	C5H10O	99.4	20.0	80 Aldrich Chemical Co.	MRI00079	A15	
15	tamoxifen	5056	CHEM10042	10540-29-1	048K1239	371.5146	C26H29NO	99	20.1	80 Aldrich Chemical Co.	MRI00079	A16	
16	Mono(2-ethylhexyl)phthalate	985	CHEM10042	4976-20-9	TX011584	278.3435	C16H22O4	99	20.3	80 Light Biologicals	MRI00079	A17	
17	Terbacil	2265	CHEM10042	5902-51-2	415-24B	216.6647	C9H13ClN2O2	99.5	20.2	80 Chem Service, Inc.	MRI00079	A18	
18	m-Dinitrobenzene	930	CHEM10042	99-65-0	TX007270	168.107	C6H4N2O4	99.9	20.7	80 Light Biologicals	MRI00079	A19	
19	2-Naphthalenesulfonic acid, 6-hydroxy-, monopotassium salt	3627	CHEM10042	833-66-9	USV4F	262.3235	C10H7KO4S	98.7	20.0	80 Sensient	MRI00079	A20	
20	L-Tryptophan	4825	CHEM10042	73-22-3	097K0119	204.2252	C11H12N2O2	100	20.0	80 Sigma	MRI00079	A21	
21	p,p'-Dichlorodiphenyl Sulfone	1140	CHEM10042	80-07-9	TX002317	287.1617	C12H8Cl2O2S	100	20.2	80 Sigma	MRI00079	A22	
22	1-heptanol	2365	CHEM10042	111-70-6	1366204	116.2013	C7H16O	99.9	20.2	80 Aldrich Chemical Co.	MRI00079	A23	
23	2,4-Diaminophenol dihydrochloride	4187	CHEM10042	137-09-7	06525MD	197.0624	C6H10Cl2N2O	98.6	19.9	80 Aldrich Chemical Co.	MRI00079	A24	
24	Dimethyltin dichloride	2895	CHEM10042	753-73-1	00119JD	219.685	C2H6Cl2Sn	99.72	20.3	80 Aldrich Chemical Co.	MRI00079	B03	
25	1-Propanamine, 3-methoxy-	3095	CHEM10042	5332-73-0	12722TD	89.1362	C4H11NO	98.9	19.8	80 Aldrich Chemical Co.	MRI00079	B04	
26	Benzene, 1-chloro-2-methyl-	2139	CHEM10042	95-49-8	11512AD	126.5835	C7H7Cl	99.64	20.1	80 Aldrich Chemical Co.	MRI00079	B05	
27	Benzofuran	129	CHEM10042	271-89-6	TX009258	118.1326	C8H6O	99.5	20	80 Sigma	MRI00079	B06	
28	alpha-Cyclodextrin	477	CHEM10042	10016-20-3	087K1343	972.8436	C36H60O30	98	20.0	80 Sigma	MRI00079	B07	
29	beta-Butyrolactone	544	CHEM10042	3068-88-0	08806AC	86.0892	C4H6O2	99.3	21.1	80 Sigma	MRI00079	B08	
30	Flutolanil	2176	CHEM10042	66332-96-5	TX011593	323.3096	C17H16F3NO2	99.5	20	80 Light Biologicals	MRI00079	B09	
31	Tris(2-chloroethyl) phosphate	1381	CHEM10042	115-96-8	07430JR	285.4898	C6H12Cl3O4P	99.07	19.9	80 Sigma	MRI00079	B10	
32	Indium trichloride	866	CHEM10042	10025-82-8	TX010854	221.177	Cl3In	99.9	20	80 Light Biologicals	MRI00079	B11	
33	N-Nitrosodiethylamine	1072	CHEM10042	55-18-5	1099224	102.135	C4H10N2O	98.45	20.1	80 Sigma	MRI00079	B12	
34	o-Toluidine	1130	CHEM10042	95-53-4	04204PC	107.1531	C7H9N	97.83	19.9	80 Sigma	MRI00079	B13	
35	Isoamyl acetate	871	CHEM10042	123-92-2	05838LN	130.1849	C7H14O2	99.3	20.0	80 Aldrich Chemical Co.	MRI00079	B14	
36	2',4',5'-Trihydroxybutyrophenone	200	CHEM10042	1421-63-2	TX009200	196.1999	C10H12O4	99.5	20	80 Sigma	MRI00079	B15	
37	o-Nitrobenzoic acid	1390	CHEM10042	83-32-7	1100559	167.1189	C7H5NO4	99.5	20.0	80 Sigma	MRI00079	B16	

2. Field names (column titles) and definitions are listed below:

1. Chemical Name
2. NTP substance identification number (SID)
3. CHEM Task No: Number assigned to the handling assignment by the NTP IMS.
4. CAS Number
5. Lot number



## Appendix 7.1 Examples of HTS Plate Maps and Structure Files.

3. DSSTox\_CID
4. DSSTox\_Generic\_SID
5. NTP\_SID
6. STRUCTURE\_Formula
7. STRUCTURE\_MolecularWeight
8. STRUCTURE\_ChemicalType
9. STRUCTURE\_TestForm\_DefinedOrganic
10. STRUCTURE\_Shown
11. TestSubstance\_ChemicalName
12. Source\_ChemicalName
13. TestSubstance\_CASRN
14. TestSubstance\_Description
15. ChemicalNote
16. STRUCTURE\_ChemicalName\_IUPAC
17. STRUCTURE\_SMILES
18. STRUCTURE\_Parent\_SMILES
19. STRUCTURE\_InChi
20. STRUCTURE\_InChiKey
21. Substance\_modify\_yymmdd
22. Note\_NTPHTS

## Appendix 7.1 Examples of HTS Plate Maps and Structure Files.

23. Aliquot\_Conc\_(mM)

24. Supplier

25. Lot\_Number

26. Purity (%)

27. NTP\_Set1

28. NTP\_SetB

29. Tox21\_duplicate

30. Tox21\_Solution\_ID

3. Definitions for fields and example structure files can be found on the DSSTox website at:  
<http://www.epa.gov/ncct/dsstox>.