Appendix 7.1

Chemistry Specifications for Chemistry Services Contractors

National Toxicology Program

Examples of HTS Plate Maps and Structure Files

September 12, 2013

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

Figure 1.



* 1. 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
		6. Molecular Wt (g/mol): Molecular weight of the chemical used to calculate the molarity of the dispensed solution.
		7. Molecular formula
		8. Purity (%): Supplier or as determined, if available.
		9. Final Conc (mM): Prepared concentration of the solution in the well.
		10. Aliquot volume (uL): Volume dispensed into the well
		11. Supplier
		12. Plate ID
		13. Plate Position: Row and column identifiers
1. Structure File
	1. A partial structure file in Excel format is shown in Figure 2.

Figure 2.



* 1. Field names (column titles) are listed below:
		1. Tox21\_ID
		2. Tox21\_RID
		3. DSSTox\_CID
		4. DSSTox\_Generic\_SID
		5. NTP\_SID
		6. STRUCTURE\_Formula
		7. STRUCTURE\_MolecularWeight
		8. STRUCTURE\_\_ChemicalType
		9. STRUCTURE\_TestedForm\_DefinedOrganic
		10. STRUCTURE\_Shown
		11. TestSubstance\_ChemcialName
		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\_yyymmdd
		22. Note\_NTPHTS
		23. Aliquot\_Conc\_(mM)
		24. Supplier
		25. Lot\_Number
		26. Purity (%)
		27. NTP\_Set1
		28. NTP\_SetB
		29. Tox21\_duplicate
		30. Tox21\_Solution\_ID
	2. Definitions for fields and example structure files can be found on the DSSTox website at: <http://www.epa.gov/ncct/dsstox>.