

Appendix B. Examples of Toxicity Screening Plate Maps and Structure Files

**Specifications for the Conduct of Chemistry Activities for Toxicology
Research Performed by the
Division of Translational Toxicology at the
National Institute of Environmental Health Sciences**

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Plate Map

Example plate maps are shown in Table B-1 and Table B-2.

Table B-1. Coded Plate

Blind-Code	Conc. (mM)	CoA Purity (%)	Determined Purity*(%)	Plate Position
2236	99.982	98.92	98.41	A1
2159	100.014	99.00	98.2	A2
2904	99.980	98.88	98.6	A3
2539	100.049	~ 99.8	NA ¹	A4
2435	100.028	97.65	99.00	A5
2310	99.816	99.60	99.1	A6
2125	100.072	99.42	99.01	A7

¹NA = not available.

Table B-2. Decoded Plate

Blind-Code	Molecular Weight	Chemical Name	CAS No.	DTXSID	Conc. (mM)	Supplier	Lot No.	CoA Purity (%)	Determined Purity*(%)	Plate Position
2236	358.47	Tetrahydrocannabinolic acid-A	23978-85-0	DTXSID30178701	99.982	KinetoChem LLC	THCAA-RD-230208	98.92	98.41	A1
2159	182.17	D-Mannitol	69-65-8	DTXSID1023235	100.014	Sigma-Aldrich	077K0166	99.00	98.2	A2
2904	314.47	Δ 9-Tetrahydrocannabinol	1972-08-3	DTXSID6021327	99.980	KinetoChem LLC	THC-RD-221109	98.88	98.6	A3
2539	183.32	Cadmium chloride	10108-64-2	DTXSID6020226	100.049	Sigma-Aldrich	03612CJ	~ 99.8	NA ¹	A4
2435	286.4	Tetrahydrocannabivarin	31262-37-0	DTXSID10893920	100.028	KinetoChem LLC	THCV-RD-230214	97.65	99.00	A5
2310	314.47	Δ 10-Tetrahydrocannabinol	95543-62-7	DTXSID401038856	99.816	KinetoChem LLC	RR-D10THC-RD-230301	99.60	99.1	A6
2125	314.47	Δ 8-Tetrahydrocannabinol	5957-75-5	DTXSID20878586	100.072	KinetoChem LLC	D8THC-RD-221109	99.42	99.01	A7

¹NA = not available.

Appendix B. Examples of Toxicity Screening Plate Maps and Structure Files

Field names (column titles) and definitions for Table B-1 and Table B-2 are listed below:

1. Blind-code (code number for aliquot used for blinded shipments)
2. Molecular weight (g/mol)
3. Chemical Name
4. CAS Number
5. DTXSID (EPA substance ID number)
6. Solution concentration (use aliquot weight if neat chemical is sent)
7. Supplier
8. Supplier Lot No. (If combined lot, use Lab-generated lot number from CH report)
9. COA Purity (%): from supplier
10. Determined purity, if available
11. Plate Position: Row and column identifiers, e.g., row A column 3 – A3

Field names (column titles) for Figure B-1 are listed below:

12. Plate
13. DTXSID
14. STRUCTURE_Formula
15. STRUCTURE_MolecularWeight
16. STRUCTURE_ChemicalType
17. STRUCTURE_TestForm_DefinedOrganic
18. STRUCTURE_Shown
19. TestSubstance_ChemicalName
20. Source_ChemicalName
21. TestSubstance_CASRN
22. TestSubstance_Description
23. ChemicalNote
24. STRUCTURE_ChemicalName_IUPAC
25. STRUCTURE_SMILES
26. STRUCTURE_Parent_SMILES
27. STRUCTURE_InChi
28. STRUCTURE_InChiKey
29. Substance_modify_YYMMDD
30. Note_NTPHTS
31. Aliquot_Conc_(mM)
32. Supplier
33. Lot_Number
34. Purity (%)

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- 35. NTP_Set1
- 36. NTP_SetB
- 37. Tox21_duplicate
- 38. Tox21_Solution_ID

