Quick Guide to Creating a Structure-Data File (SD File) for Type II Drug Master File (DMF) Submissions

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Introduction

The pharmaceutical industry may now submit structures to the Agency through the Electronic Common Technical Document (eCTD) as a single Structure-Data File (SD File) with standardized data fields meeting the Agency's cheminformatics and review needs. The SD File is acceptable in all of Module 3.[1] This guide is designed to aid in the creation of an SD File. It is not intended to be a comprehensive review of the SD File format. Extensive technical details on the file format can be found on the internet.[2]

What is an SD File?

- An SD File is a chemical structure-data file in MOL connection table format and can list one or more chemical structures (See Figure 1). The MOL connection table format describes the chemical structure using a block of text that lists the atoms, bonds, connectivity, and coordinates. Associated data can be appended to the MOL connection table. [1] Chemical software translate the text into an image of the chemical structure and places the data into a table (See Figure 2).
- SD Files are commonly called SD File or SDF.
- The SD File extension is .sdf.

```
Acetamide



  4  3  0  0  0  0  0  0  0  0999 V2000
    0.0000   -0.2062    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.0000    0.6188    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.7145   -0.6188    0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
    0.7145   -0.6188    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  2  0  0  0  0
  1  3  1  0  0  0  0
  1  4  1  0  0  0  0
M  END
>  <Notes>
Applicants can include text
$$$$
```

Figure 1. Example contents of an SD File

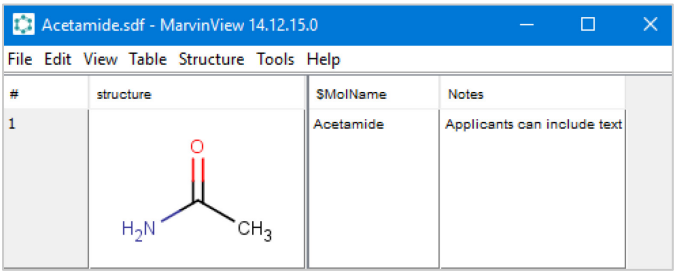


Figure 2. Chemical software can interpret an SD File and translate the content into a graphical chemical structure and data table.

Guidelines for creating an SD File for Type II DMF submissions

- Use V2000 format.
- Create one SD file that contains all chemical structures.
- Place in Module 3 section 3.2.S.3.2.
- You are encouraged to use and fill-in the blank SD File template attached to this document for your submission.
- The file name should include the DMF number (e.g., MF012345) and name of the Drug Substance.
- **Only include chemical structures that undergo a hazard assessment evaluated by (Q)SAR to predict potential bacterial mutagenicity.**
- Create one SD file and include chemical structures of the following:
    - Drug substance(s)
    - Process impurities
    - Intermediates
    - Degradants
    - Starting materials.
- **EXCLUDE** reagents and solvents. Refer to FDA Guidance for Industry Q3A, 2008,[3] for definitions.
- Verify that the ID and CAS number are correct and that the structures have rendered accurately.
- Verify that the application number (i.e., MF012345) listed in the SD File is the same as the application number of the submission.
- Ensure the file extension is .sdf.

Include the following columns named in this order (See Figure 3 for rendering example):

Column Name:	Data Item
Structure	Chemical structure
Name	Chemical name (common or IUPAC) as referenced in the DMF
CAS	Include if available. CAS are available from SciFinder - https://scifinder.cas.org and PubChem https://pubchem.ncbi.nlm.nih.gov/.
Role	Examples of roles are drug substance(s), process impurity, intermediate, degradant, metabolite, or starting material. Other appropriate descriptions are allowed if necessary.
ID	Include if available. Include unique company codes or code names used throughout the SD File and DMF submission. This will be used for cross-referencing structures in the file and other documents (e.g., Structure UVX123, CompanyXYZ010102, etc.).
UNII	Include if available. UNII may be found at https://precision.fda.gov/uniisearch and https://gsrs.ncats.nih.gov/ginas/app/beta/.
Application Number	Include the "MF" prefix before the DMF number. Include leading zero(s). Exclude dashes and spaces (e.g., "MF012345").
Notes	Include if needed. Notes specify/qualify something about the substance that is not easily discernable from the structure alone. For example, specifying that the chemical substance has axial chirality and is the "R" stereoisomer.

Software to create an SD File

Open-source and/or commercial software can be used to help you create an SD File. The following are examples of software that can aid in creating or editing an SD File. Note that this list is not exhaustive, and many other tools may be used in creating and editing these files.

- Open Babel
- DataWarrior
- KNIME SDF Writer
- ChemAxon Marvin
- ChemOffice ChemFinder
- Instem Leadscope SDF Editor
- Molecular Operating Environment
- RDKit
- CDK

Sample instructions to create an SD File using DataWarrior or Instem Leadscope SDF Editor

DataWarrior Example

The following provides sample steps for creating an SD File using DataWarrior.

1. Open DataWarrior.
2. Click File → Open. Select File name: TemplateSDF_ApplicationTypeXXXXXX_DrugSubstanceName.sdf.
3. Go to Data in the top menu bar → Click on Add Empty Rows… Count of new rows: Enter the number of rows needed (total number of rows is equal to number of chemical structures. Click OK.
4. Under the "Structure" column, double-click a structure cell to draw a chemical structure. Click OK.
5. Alternatively, you can copy a SMILES-string, molfile contents, ChemDraw or Accelrys Draw object. Then right-click an empty cell in the structure column, select "Paste Into Table."
6. Double click any cell to add or edit data. Click OK.
7. Repeat steps 4 to 6 until all chemical structures and data are entered.
8. If necessary to add columns, go to Data in the top menu bar →Click on Add Empty Columns…
    - Click on drop down arrow of "Column Type" → Select either Text for data or Structure for chemical structures.
    - In Column Name text field, enter the name of the column.
    - Click "Add Column."
    - Repeat if needed for additional columns.
    - Once all columns are defined, click "OK."
9. **Go to File → Save Special… → SD-File**
    - File name: SDF_MF######_API_Name.sdf, click "Save."
    - A "Save SD-File" window will open. Select the following
        - Structure Column: **Structure**
        - SD-file version: **Version 2**
        - Atom Coordinates: **2D**
        - Compound name column: Name
    - Click "OK."

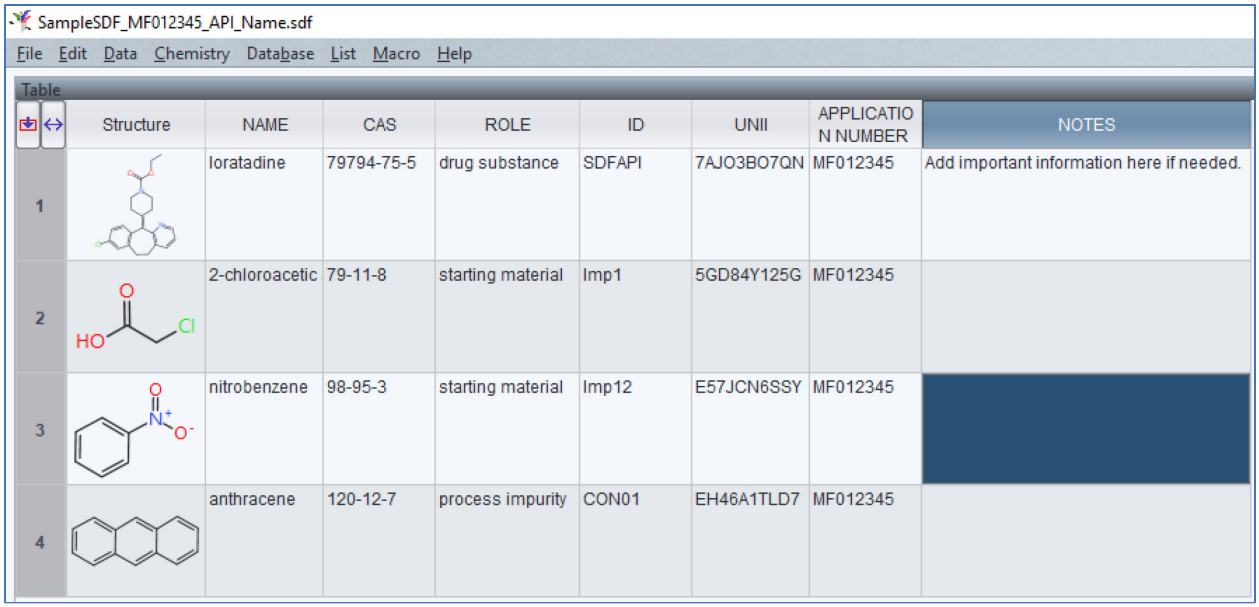


Figure 3. Screenshot from DataWarrior of chemical structures and associated data in an SD File.

Leadscope Example

The following provides sample steps for creating an SD file Leadscope Structure SDF Editor.

1. Open Leadscope Structure SDF Editor software.
2. Go to File → Open SDF/Mol/SMILES
   Select File name:
   TemplateSDF_ApplicationTypeXXXXXX_DrugSubstanceName.sdf
3. Go to File → Draw new structure…
4. Leadscope Structure Editor window will open.
   - Use the tools to draw the structure.
   - Enter a name in the Name field located at the bottom of the window.
5. Go to Tools on the menu bar → Select Validate → Select the options for validation: All Checks. → Click Ok.
6. Address all validation errors. When finished, close the window by clicking the "X" in the upper right-hand corner of the Structure Editor window.
7. Window will open and ask, "Would you like to keep the structural changes?" Click Yes.
8. Repeat steps 3 to 7 for additional chemicals.
9. Double-click a cell to enter or edit data. The cursor will blink. Type in data. Press enter when done.
10. To add another column, right-click any column header → Add property → type name of property (e.g., NAME). Repeat for additional columns.
11. Go to File → Save As… →
    - File name: SDF_MFXXXXXX_API_Name.sdf
    - Files of type: SD File (.sdf)
12. Click Save.

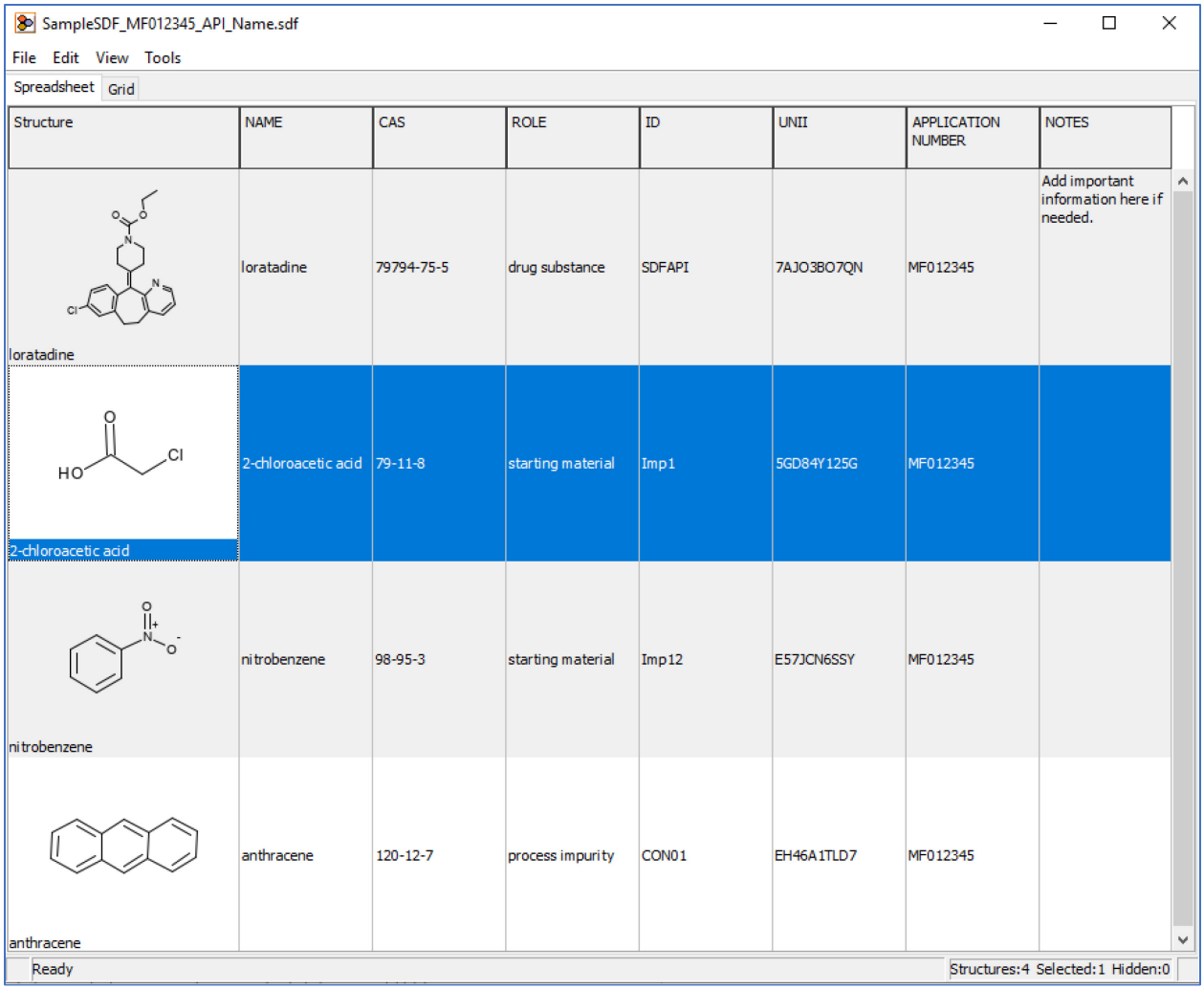
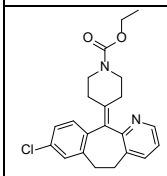
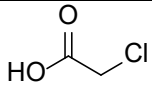
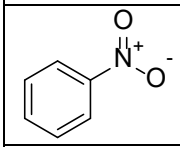
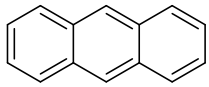


Figure 4. Screenshot of Leadscope SDF Editor of chemical structures and associated data in an SD File.

Text format of column names and data when viewed using an SD File viewer. An example of the raw ASCII text of the SD File is available in the Appendix and attached.

Structure	NAME	CAS	ROLE	ID	UNII	APPLICATION NUMBER	NOTES
	loratadine	79794-75-5	drug substance	SDFAPI	7AJO3BO7QN	MF012345	Add important information here if needed.
	2-chloroacetic acid	79-11-8	starting material	Imp1	5GD84Y125G	MF012345	
	nitrobenzene	98-95-3	starting material	Imp12	E57JCN6SSY	MF012345	
	anthracene	120-12-7	process impurity	CON01	EH46A1TLD7	MF012345	

Recommendations for special chemical structure scenarios

For special chemical structure scenarios, such as but not limited to, salts, mixtures, 3-D configurations, isotopes, or stereochemistry, please use the guidelines below.

Mixtures

For substances that have a UNII and/or CAS registry number but have no appropriate single simple chemical structure, the structure component of the record can be left blank while the UNII and/or CAS data item are filled (e.g., Xylenes).

Atom Notations

- **Exclude** query attributes for atoms or bonds – e.g., do not include X's, star atoms, etc. The double-either bond is allowed when necessary.
- **Exclude** "Sgroups" (e.g., monomer brackets, SRU designations brackets, data brackets, etc.) within the MOLfile. The one exception is that "multiple group" Sgroup bracket types (i.e., "MUL" groups) can be used to represent stoichiometry of salts and hydrates.
- **Exclude** "super atoms" where shorthand notations like "NO2" and "Ph" are used to specify functional groups. Every atom should be specified in isolation without aliases or groupings.
- **Exclude** annotations/embedded text properties in the MOL file to indicate stereochemistry.

Isotopes

Include specific isotopes only if structure is isotopically labelled or isotopically enriched. The "M ISO" attribute of the MOLfile should be used to encode this information when needed.

Stereochemistry

- Include all **known** stereochemistry and indicate where stereochemistry is present using stereo bonds (wedge  and hash  bonds).
- Stereo bonds should point to chiral atoms. See GSRS levomenthol example.
- Include stoichiometry explicitly if known for salts and solvates.
- If stereochemistry is unknown, explicitly write in the "NOTES" column that the stereochemistry is *unknown.*
- If stereochemistry is relative, explicitly write in the "NOTES" column that the stereochemistry is *relative* (i.e., relative stereochemistry indicates that the stereochemistry is known and the identifiers (name, CAS, or UNII) designate the substance is racemic or includes its enantiomer). See GSRS racementhol example.
- If double bond geometry is known, it should be depicted by appropriate atom coordinates. The implicit E or Z configuration of the depicted 2D coordinates will be assumed to be intentional. See GSRS 2-BUTENE, (E)- and 2-BUTENE, (Z)- examples.
- If double bond geometry is unknown or is a mixture, the double-either bond should be used OR the atoms should be arranged in a colinear fashion which does not imply E/Z designation.

Configurations

- Depict explicit Kekulé forms of molecules using single and double bonds instead of using aromatic bond types.
- Draw the prevalent tautomeric form of the compound.
- 2D representations are both adequate and preferred to 3D representations.

Mixtures, salts, or coordination complexes

- Impurities should be represented as free acids or bases. Do not represent as salts.
- Drug substances that are truly salts (e.g., Na^+, H^+, $NH4^+$, Cl^-) can be represented as salts.
- Amine salts other than quaternary amines should be represented uncharged as hydrochlorides, hydrobromides etc. Metal salts can be charged and should always be charged balanced.
- Where possible, each structure should contain only one covalently connected entity. Multiple covalent entities within one record are allowed for the case of salts, hydrates, coordination complexes and inorganic substances.
- A mixture of organic substances should be presented in separate records.

Carbohydrates, steroids, cyclic structures

- Use planar drawings for cyclic structures and ring systems. See GSRS cholesterol and tetracycline example.
- Use stereo bonds (wedge and hash bonds) to indicate stereochemistry instead of Fischer, Haworth, and chair projections. See GSRS D-galactose example.
- Use explicit hydrogens to specify stereochemistry on rings.

Proteins and peptides

- Do not include collapsed amino acid notations (single letter or 3 letter) in the structure. Instead have the amino acids expanded without groupings.
- Do not include aliases for atoms (e.g., “Me” for methyl).
- See GSRS zendusortide and zendusortide structure example.
- For complex proteins, peptides, and substances with unnatural amino acids that require additional data elements to describe or are difficult to represent with a single chemical structure, please contact FDA-SRS@fda.hhs.gov. Include the application type and number or reference, details of the amino acid sequence, disulfide bonds, glycosylation sites, amino acid site and type modifications/ mutation, and chemical structure of unnatural amino acids in the correspondence.

Additional support

- A **sample SD File** (SampleSDF_MF012345_API_Name.sdf) is available in the attachments.
- An **SD File template** (TemplateSDF_ApplicationTypeXXXXXX_DrugSubstanceName.sdf) is attached for your convenience. The column names are prepopulated to promote data harmonization. We encourage you to import into a cheminformatics software that is

capable of reading and editing SD Files. This will enable you to populate with chemical structures and data that will undergo a hazard assessment.

- FDA GSRS enables an efficient and accurate exchange of information on substances through their UNII, which can be generated prior to submissions and at any time in the regulatory life cycle.
    - To search for a substance by name, use FDA GSRS UNII Search Service, https://precision.fda.gov/uniisearch.
    - To search for a substance by chemical structure, use the public NIH GSRS database, https://gsrs.ncats.nih.gov/ginas/app/beta/.
    - The Bulk Search tool is available for searching multiple substances at a time by name (common or IUPAC), CAS, InChIKey, and UNII, https://gsrs.ncats.nih.gov/ginas/app/beta/bulk-search.
    - For more information about GSRS database and the UNII, visit FDA GSRS Homepage or watch GSRS' Grand Round webcast.
- For general questions on formatting or submitting SD Files, please contact FDA-SRS@fda.hhs.gov.
- For trouble submitting SD Files related to DMF applications, please contact DMFOGD@fda.hhs.gov.
- If you have questions for CDER related to eCTD submissions, please contact the CDER Electronic Submission (ESUB) Support Team at esub@fda.hhs.gov.

FAQ

Q. I need a UNIII and cannot find the UNII for my substance in GSRS.
A. Include, if available, otherwise a UNII will be generated by the Agency after submission.

Q. Should reagents and solvents be included in the SD File?
A. No.

Q. Are reagents and solvents also starting materials?
A. No. According to FDA Guidance for Industry Q3A, 2008:[3]

> A starting material is incorporated as a significant structural fragment into the structure of the drug substance. Significant structural fragment in this context is intended to distinguish starting materials from reagents, solvents, or other raw materials. Commonly available chemicals used to create salts, esters, or other simple derivatives should be considered reagents.
>
> **Starting Material**: A material used in the synthesis of a new drug substance that is incorporated as an element into the structure of an intermediate and/or of the new drug substance.
>
> **Solvents** are inorganic or organic liquids used as vehicles for the preparation of solutions or suspensions in the synthesis of a new drug substance.
>
> **Reagent**: A substance other than a starting material, intermediate, or solvent that is used in the manufacture of a new drug substance
>
> Guidance for Industry Q3A Impurities in New Drug Substances, 2008. https://www.fda.gov/regulatory-information/search-fda-guidance-documents/q3ar-impurities-new-drug-substances (accessed February 1, 2024).

Q. I previously submitted a substance with a UNII. However, I cannot find the UNII in the GSRS database.
A. It is possible the UNII is not public. Please move forward with submitting the SD File with the UNII you have on file for your substance.

Q. Multiple UNIIs come up when I search for an ingredient by CAS (e.g., 9004-65-3, Hypromellose). Which one should I pick?
A. UNIIs were created to meet FDA's regulatory needs. Therefore, other identifiers or monographs may not provide enough information to point to the precise UNII. Check the technical data sheet or safety data sheet for the composition of the ingredient, physical and chemical properties, or product name. Include the data sheet when contacting FDA-SRS@fda.hhs.gov for help.

Q. Where should I put the SD File in the eCTD?
A. Chemical impurities that undergo a hazard assessment evaluated by (Q)SAR to predict potential mutagenicity should be placed in Module 3 section 3.2.S.3.2 of the eCTD.

Q. We tabulated all chemical structures, UNII, and CAS in ChemDraw (.cdx file) and converted to an SD File (.sdf). However, the SD File is missing data. Why?
A. ChemDraw will only create an SD File with structures regardless of any additional text that may be in the .cdx file. We recommend generating the SD file using the software listed above.

Q. Regarding using SD Files to submit the data of chemical structures, is the submission of the SD file now an officially mandatory requirement?
A. Submitting an SD File with your submission is not required. However, submitting one, especially if asked to do so, will aid in an efficient review of the DMF. SD Files are used to support (Q)SAR and computational toxicology assessments.

Q. Should the SD File be attached to a Word or PDF file (in the corresponding section of the DMF). Or do we convert the file to .txt and paste it into the corresponding section in Word?
A.

- The SD File is a standalone document.
- DO NOT convert the file extension from .sdf to .txt
- DO NOT convert the SD File to a PDF.
- DO NOT embed nor copy-paste the contents of the SD file into a Word document.
- Ensure the SD File is mapped to the XML file index or else an error message will be generated. However, the error message will not prevent you from uploading your submission. For help mapping the file, please contact CDER Electronic Submission (ESUB) Support Team at esub@fda.hhs.gov.

Q. I created an SD File in DataWarrior and attempted to upload it to the eCTD. However, the eCTD software is unable to support the DataWarrior file.
A. Please note that DataWarrior by default saves files as a ".dwar" file format. Please make sure you select "Save Special – SD-File" when saving. Refer to the DataWarrior Example above.

References

1. 3.3.3 Structure-Data Files, eCTD Technical Conformance Guide v1.8. U.S. Department of Health and Human Services, Food and Drug Administration, Center for Drug Evaluation and Research, Center for Biologics Evaluation and Research, November 2022, page 13-14, https://www.fda.gov/drugs/electronic-regulatory-submission-and-review/electronic-common-technical-document-ectd (accessed February 1, 2024).

2. Dalby A, et al. Description of several chemical structure file formats used by computer programs developed at Molecular Design Limited. J. Chem. Inf. Comput. Sci. 1992, 32, 3, 244–255. https://pubs.acs.org/doi/10.1021/ci00007a012.

3. Guidance for Industry Q3A Impurities in New Drug Substances. U.S. Department of Health and Human Services, Food and Drug Administration, Center for Drug Evaluation and Research, Center for Biologics Evaluation and Research, November 2012. https://www.fda.gov/regulatory-information/search-fda-guidance-documents/q3ar-impurities-new-drug-substances (accessed February 1, 2024).

Appendix: Example of ASCII text of an SD File.

```
loratadine


 27 30  0  0  0  0  0  0  0  0999 V2000
    0.0000   -0.0000   -0.0000 Cl  0  0  0  0  0  0  0  0  0  0  0  0
    1.4087    0.4656   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.4831   -0.5253   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.7310    1.9578   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.8917   -0.0597   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.1396    2.4234   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.2141    1.4325   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.8109   -1.2057   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.5392    2.1130   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    6.2912   -1.1818   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    6.8643    1.4803   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.5153    3.6410   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    7.2104    0.0119   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    7.9387    2.5189   -0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
    6.7926    4.4051   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.1902    4.4051   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    8.6191   -0.4059   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.3473    2.1011   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    6.7687    5.9331   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.1663    5.9331   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    9.6935    0.6327   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.4437    6.7091   -0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
    5.4198    8.2371   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    4.0947    9.0131   -0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    6.6971    9.0131   -0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    6.6732   10.5411   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    7.9506   11.3171   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0  0  0  0
  2  3  2  0  0  0  0
  2  4  1  0  0  0  0
  3  5  1  0  0  0  0
  4  6  2  0  0  0  0
  5  7  2  0  0  0  0
  5  8  1  0  0  0  0
  7  9  1  0  0  0  0
  8 10  1  0  0  0  0
  9 11  1  0  0  0  0
  9 12  2  0  0  0  0
 10 13  1  0  0  0  0
 11 14  1  0  0  0  0
 12 15  1  0  0  0  0
 12 16  1  0  0  0  0
 13 17  1  0  0  0  0
 14 18  2  0  0  0  0
 15 19  1  0  0  0  0
 16 20  1  0  0  0  0
 17 21  2  0  0  0  0
 19 22  1  0  0  0  0
 22 23  1  0  0  0  0
 23 24  2  0  0  0  0
 23 25  1  0  0  0  0
 25 26  1  0  0  0  0
 26 27  1  0  0  0  0
  6  7  1  0  0  0  0
 11 13  2  0  0  0  0
 18 21  1  0  0  0  0
 20 22  1  0  0  0  0
M  END
>  <NAME>
loratadine

>  <CAS>
79794-75-5
```

```
>  <ROLE>
drug substance

>  <ID>
SDFAPI

>  <UNII>
7AJO3BO7QN

>  <APPLICATION NUMBER>
MF012345

>  <NOTES>
Add important information here if needed.

$$$$
2-chloroacetic acid


  5  4  0  0  0  0  0  0  0  0999 V2000
    0.0000   -0.0000   -0.0000 Cl  0  0  0  0  0  0  0  0  0  0  0  0
   -1.3035   -0.7281   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.6070    0.0352   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.6305    1.5384   -0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   -3.9105   -0.6929   -0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0  0  0  0
  2  3  1  0  0  0  0
  3  4  2  0  0  0  0
  3  5  1  0  0  0  0
M  END
>  <NAME>
2-chloroacetic acid

>  <CAS>
79-11-8

>  <ROLE>
starting material

>  <ID>
Imp1

>  <UNII>
5GD84Y125G

>  <APPLICATION NUMBER>
MF012345

>  <NOTES>


$$$$
nitrobenzene


  9  9  0  0  0  0  0  0  0  0999 V2000
    0.0000   -0.0000   -0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   -0.0235   -1.4792   -0.0000 N   0  0  0  0  0  0  0  0  0  0  0  0
    1.2562   -2.1954   -0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3501   -2.1954   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.6767   -1.4205   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3736   -3.6746   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.0033   -2.1367   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.7002   -4.3907   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -4.0268   -3.6159   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  2  0  0  0  0
  2  3  1  0  0  0  0
  2  4  1  0  0  0  0
  4  5  2  0  0  0  0
  4  6  1  0  0  0  0
```

```
  5  7  1  0  0  0  0
  6  8  2  0  0  0  0
  7  9  2  0  0  0  0
  8  9  1  0  0  0  0
M  CHG  2   2   1   3  -1
M  END
>  <NAME>
nitrobenzene

>  <CAS>
98-95-3

>  <ROLE>
starting material

>  <ID>
Imp12

>  <UNII>
E57JCN6SSY

>  <APPLICATION NUMBER>
MF012345

>  <NOTES>


$$$$
anthracene


 14 16  0  0  0  0  0  0  0  0999 V2000
    0.0000   -0.0000   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -0.0236   -1.4882   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.2874    0.7795   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3347    0.7795   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.2638   -2.2087   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -1.3583   -2.2087   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.5749    0.0591   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.6694    0.0591   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.5512   -1.4292   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
   -2.6930   -1.4292   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.8623    0.8386   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.8387   -2.1497   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.1497    0.1181   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    5.1261   -1.3701   -0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0  0  0  0
  1  3  1  0  0  0  0
  1  4  2  0  0  0  0
  2  5  1  0  0  0  0
  2  6  2  0  0  0  0
  3  7  2  0  0  0  0
  4  8  1  0  0  0  0
  5  9  2  0  0  0  0
  6 10  1  0  0  0  0
  7 11  1  0  0  0  0
  9 12  1  0  0  0  0
 11 13  2  0  0  0  0
 12 14  2  0  0  0  0
  7  9  1  0  0  0  0
  8 10  2  0  0  0  0
 13 14  1  0  0  0  0
M  END
>  <NAME>
anthracene

>  <CAS>
120-12-7

>  <ROLE>
process impurity
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>  <ID>
CON01

>  <UNII>
EH46A1TLD7

>  <APPLICATION NUMBER>
MF012345

>  <NOTES>


$$$$
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