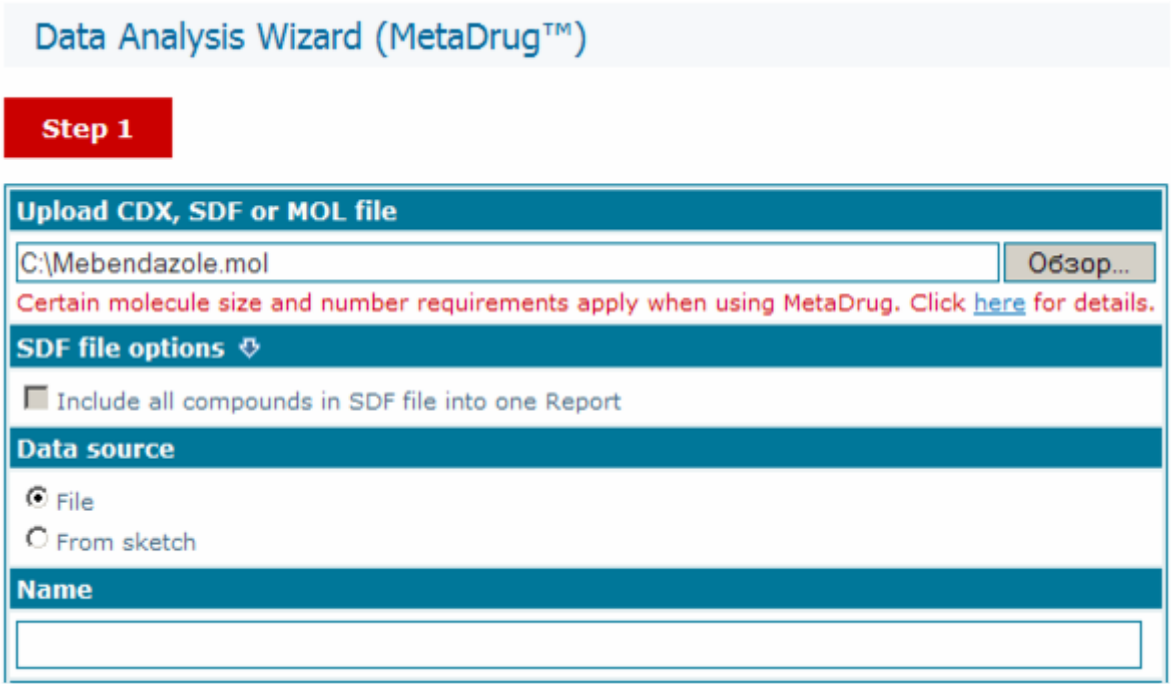
How to Upload Structures From File (MOL, SDF, CDX)

For MetaDrug™ analysis a single chemical compound can be in one of the following file formats:

- *MOL* (or MDL Molfile). In MOL file the first line (header) becomes the name of the chemical compound in the MetaDrug™ report and the name of the file becomes the name for the MetaDrug™ report itself.
- *CDX* (ChemDraw eXchange file). It contains description of a structure of single chemical compound. Typically, a name of the file is a compound name and is used by default as the name for the MetaDrug™-generated report.

In order to upload a single structure, browse for a MOL or CDX file on your computer (Figure 1), and select it. Optionally, to change the default name of the report derived from the file, a user can enter a custom name for the report in the **Name** field. This will be the name of the report that appears in the **MY STRUCTURES** folder of the Data manager.

Figure 1. Upload a MOL file to MetaDrug™



A chemical compound database can be uploaded into MetaDrug™ in the form of a SDF file. In SDF file each individual compound description has the same format as for MOL files, typically starting with the header containing the compound name. A delimiter $$$$ is used to separate the compounds from each other in one file. A feature of SDF file is the possibility of storing multiple associated data items (IDs, properties, activities) in the data fields.

MetaDrug™ splits the SDF file and calculates an individual Report for every compound in SDF file. Each Report is named after the chemical compound from its header and is placed it into the newly created folder named according the name of the SDF file. Alternatively, a single Report may be generated for all compounds in the SDF file using option **Include all compounds from SDF file into one Report** (Figure 1). The Report will be named according to the name of the file and the name of each compound in the report is obtained from the header of the compound description. The name of the Report can be altered by entering the custom name in the **Name** field.

A name of the chemical compound in the Report can also be derived from the data fields. Clicking an arrow icon by the **SDF file options** results (Figure 2) in the analysis of the SDF file data fields and opens a pane displaying all the fields. Any field can be selected to become the name of the chemical in the Report. In case when the SDF file is split it will also become the name of the Report itself.

Figure 2. **Upload a SDF file to MetaDrug™ and select the name from the data field**