# ScreenMatcher Program Manual

Guide to convert screen files to different format

*Software reviewer version

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# Manual for using the ScreenMatcher program

## A. Default Output File option

The default output file option only requires one input file and the output file generated is the format used by the analysis programs.

1. To run the program, go to the link: http:// http://datamedia.cs.uah.edu/screenmatcher )
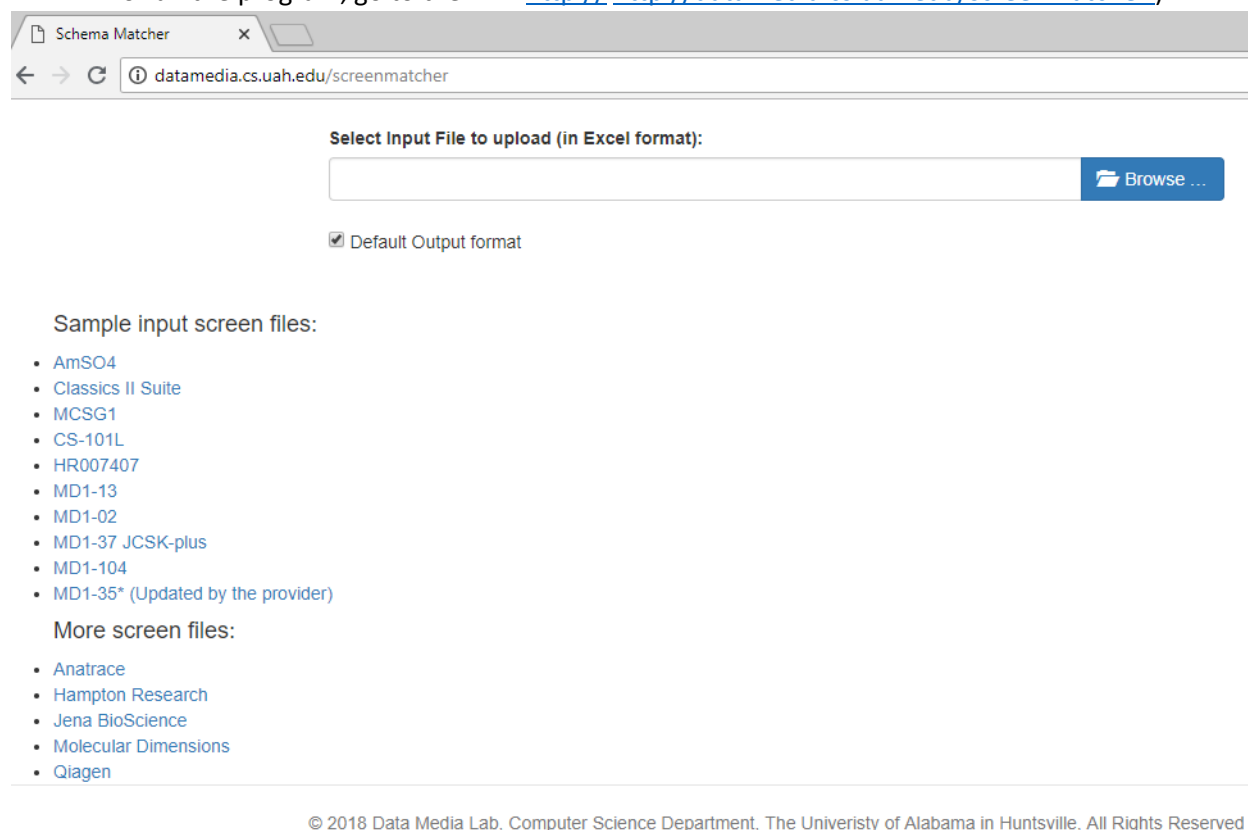


*Figure 1: Home page of the application*

Figure 1 shows the home page of the ScreenMatcher web tool. The main UI includes input screen file upload box at the top and some sample screen file in the left button.

The sample screen files are directly linked to their provider website. The users also could use their own screen file as well (in Excel format).

2. The home page of the application shows a file upload box. Click on "Browse" and search for the input screen file to upload. Once the file is chosen, you can Remove, Upload or Browse for another file. Click on "Upload" to upload the file (see Figure 2).



*Figure 2: Options after choosing file*

3. Once the file is uploaded, the matches found by the program are displayed as a table. The table contains a checkbox which enables you to select or deselect the given match, the input column which is the column number indicator in the excel file (A, B, C,...), the input header which is the column name of the input header and the corresponding matched intermediate header (see Figure 3).
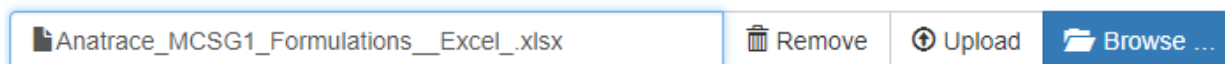
Choose Matches for Anatrace_MCSG1_Formulations-Excel.xlsx

| | Column | Input Header | Intermediate Header |
|---|---|---|---|
| ☑ | Select All | | |
| ☑ | B | Well | well_id |
| ☑ | C | [Salt] | salt_conc1 |
| ☑ | D | [Salt] units | salt_unit1 |
| ☑ | E | Salt | salt_name1 |
| ☑ | F | [Buffer] | buffer_conc |
| ☑ | G | [Buffer] units | buffer_unit |
| ☑ | H | Buffer | buffer_name |
| ☑ | J | pH | ph |
| ☑ | K | [PPT1] | precipitant_conc1 |
| ☑ | L | [PPT1] Units | precipitant_unit1 |
| ☑ | M | Precipitant 1 | precipitant_name1 |
| ☑ | N | [PPT2] | precipitant_conc2 |
| ☑ | O | [PPT2] Units | precipitant_unit2 |
| ☑ | P | Precipitant 2 | precipitant_name2 |

Add More

Accept

*Figure 3: Display and Choose Matches page*

4. You can click on the checkboxes of each match to select or deselect the matches see Figure 3).
5. You can also add new matches by clicking on the "Add More" button. After clicking on this button, two dropdown boxes are displayed: one contains the list of input headers and the other contains the list of intermediate headers. You can choose any input header and choose corresponding intermediate header to match with that input header. If you want to remove this additional match, click on the "Remove" button beside the match. Click on the "Add More" button add another match (see Figure 3 & 4).

*Figure 4: Choose additional matches from dropdown menu*

6.  Once you are done selecting the matches, click on the "Accept" button (see Figure 4).
7.  The next page shown is to add display names for unseen chemicals (see Figure 5). If no unseen chemicals are found in the input screen file, then this page is skipped (see step 11).



*Figure 5: Select display names for unseen chemicals*

8.  This page displays the IUPAC name for a chemical and a dropdown box with the list of possible names for the chemical (default selection is the IUPAC name itself). For each chemical, choose a display name from the dropdown list. If you wish to add a name not mentioned in the dropdown list, choose the "Other" option in the dropdown menu and a text box will appear. Type the display name for the chemical in the text box (see Figure 5).
9.  There is a "Skip now" checkbox to the right of every dropdown button which is checked by default in order to skip entering display names for selected chemicals. If it is checked, the

display name for that chemical is not saved to database and will be asked next time. The checkbox is automatically unchecked when the selection of the dropdown changes and can also be changed manually by clicking on it (see Figure 5).

10. After choosing display names for all chemicals, click on the "Submit" button (see Figure 5).
11. Then the output file will be written to the output folder inside the ScreenMatcher folder. You can also use the "Download file" button to directly download the output file to a desired location. You can continue to convert another file by go to this home page http:// http://datamedia.cs.uah.edu/screenmatcher and repeating above steps.

** If using web browser backward navigation, make sure that you refresh the ScreenMatcher home page.

**Output file is ready:** [ Download File ]

Matches for Anatrace_MCSG1_Formulations-Excel

| Input Column | Input Header | Intermediate Header |
|---|---|---|
| B | Well | well_id |
| C | [Salt] | salt_conc1 |
| D | [Salt] units | salt_unit1 |
| E | Salt | salt_name1 |
| F | [Buffer] | buffer_conc |
| G | [Buffer] units | buffer_unit |
| H | Buffer | buffer_name |
| J | pH | ph |
| K | [PPT1] | precipitant_conc1 |
| L | [PPT1] Units | precipitant_unit1 |
| M | Precipitant 1 | precipitant_name1 |
| N | [PPT2] | precipitant_conc2 |
| O | [PPT2] Units | precipitant_unit2 |
| P | Precipitant 2 | precipitant_name2 |

*Figure 6: Final matches and Output file download page*

| | A | B | C | D | E | F | G | H | I | J | K | L | M | N | O | P | Q | R | S | T | U | V |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | Well_Id | B_Anion | B_Cation | Ph | B_Conc | C1_Anion | C1_Cation | C1_Conc | C1_M | C1_Ph | C2_Anion | C2_Cation | C2_Conc | C2_M | C2_Ph | C3_Anion | C3_Cation | C3_Conc | C3_M | C3_Ph | C4_Anion | C4_C |
| 2 | a1 | hepes | | 7.5 | 0.1 | peg 8000 | | 20 | | | | | | | | | | | | | | |
| 3 | a2 | ches | | 9.5 | 0.1 | peg 3000 | | 30 | | | | | | | | | | | | | | |
| 4 | a3 | na2hpo4/kh2po4 | | 6.2 | 0.1 | peg 8000 | | 10 | | | chloride | sodium | | 0.2 | | | | | | | | |
| 5 | a4 | tris | | 7 | 0.1 | chloride | sodium | | 2.5 | | chloride | magnesium | | 0.2 | | | | | | | | |
| 6 | a5 | acetate | sodium | 4.5 | 0.1 | sulfate | ammonium | | 1.26 | | chloride | sodium | | 0.2 | | | | | | | | |
| 7 | a6 | bis-tris | | 5.5 | 0.1 | peg 3350 | | 25 | | | sulfate | ammonium | | 0.2 | | | | | | | | |
| 8 | a7 | bis-tris | | 5.5 | 0.1 | peg 3350 | | 25 | | | chloride | magnesium | | 0.2 | | | | | | | | |
| 9 | a8 | tris | | 7 | 0.1 | peg mme 2000 | | 20 | | | | | | | | | | | | | | |
| 10 | a9 | hepes | | 7.5 | 0.1 | peg 3350 | | 25 | | | chloride | magnesium | | 0.2 | | | | | | | | |
| 11 | a10 | hepes | | 7.5 | 0.1 | ppg p400 | | 28 | | | chloride | calcium | | 0.2 | | | | | | | | |
| 12 | a11 | mes | | 6.5 | 0.1 | peg 4000 | | 10 | | | chloride | magnesium | | 0.2 | | | | | | | | |
| 13 | a12 | tris | | 8.5 | 0.1 | peg 4000 | | 20 | | | chloride | calcium | | 0.2 | | | | | | | | |
| 14 | b1 | mes | | 6.5 | 0.1 | peg 4000 | | 20 | | | chloride | sodium | | 0.6 | | | | | | | | |
| 15 | b2 | bis-tris | | 5.5 | 0.1 | peg 3350 | | 25 | | | chloride | sodium | | 0.2 | | | | | | | | |
| 16 | b3 | bis-tris | | 5.5 | 0.1 | peg 3350 | | 25 | | | acetate | ammonium | | 0.2 | | | | | | | | |
| 17 | b4 | bis-tris | | 6.5 | 0.1 | peg 3350 | | 25 | | | chloride | magnesium | | 0.2 | | | | | | | | |
| 18 | b5 | tris | | 8.5 | 0.1 | peg 3350 | | 25 | | | chloride | magnesium | | 0.2 | | | | | | | | |
| 19 | b6 | mes | | 6 | 0.1 | peg 8000 | | 25 | | | diacetate hydra | calcium | | 0.2 | | | | | | | | |
| 20 | b7 | citrate | sodium | 5.6 | 0.085 | peg 4000 | | 25.5 | | | acetate | ammonium | | 0.17 | | glycerol | | 15 | | | | |
| 21 | b8 | tris | | 8.5 | 0.085 | peg 4000 | | 25.5 | | | acetate | sodium | | 0.17 | | glycerol | | 15 | | | | |
| 22 | b9 | | | | | peg 3350 | | 20 | | | chloride | magnesium | | 0.2 | | | | | | | | |
| 23 | b10 | tris | | 8.5 | 0.08 | peg 4000 | | 24 | | | chloride | magnesium | | 0.16 | | glycerol | | 20 | | | | |
| 24 | b11 | tris | | 8.5 | 0.1 | peg 8000 | | 20 | | | chloride | magnesium | | 0.2 | | | | | | | | |

*Figure 7: Example of Output file from Anatrace MCSG screen*

## B. Non-Default Output File option

The non-default output option allows the user to specify the format for the output file as well. The sample output screen file can be uploaded along with the input screen file and the output of the program will be the file with data from the input file in the sample output file format.

1. To run the program, go to the link: http:// http://datamedia.cs.uah.edu/screenmatcher )
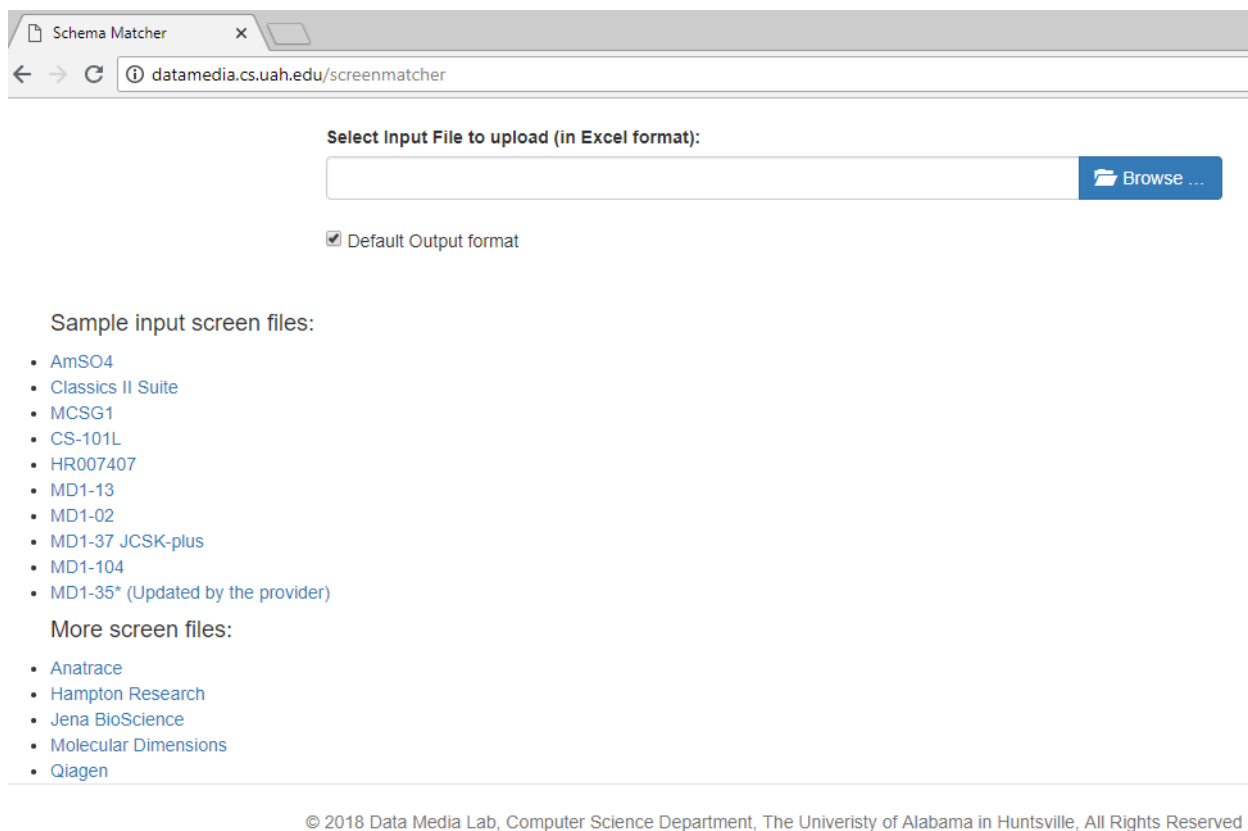


*Figure 6: Home page of the program*

Figure 8 shows the home page of the ScreenMatcher web tool. The main UI includes input screen file upload box at the top and some sample screen file in the left button.

The sample screen files are directly linked to their provider website. The users also could use their own screen file as well (in Excel format).

2. The home page of the application shows a file upload box. Click on "Browse" and search for the input screen file to upload. Once the file is chosen, you can Remove, or Browse for another file.
3. Below the file upload box, there is a checkbox for "Default Output format" which is checked by default. Uncheck the box and a second file upload box will appear for the output file. Select the sample screen file for the output format and click on Upload.
   *Note: in this version, by click on Upload button, both input and sample output file will be uploaded.

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**Select Input File to upload (in Excel format):**

| Anatrace_MCSG1_Formulations__Excel_.xlsx | 🗑 Remove | ⊕ Upload | 📂 Browse ... |

☐ Default Output format

**Select sample Output File (for output format) to upload (in Excel format):**

| MD1_02 Structure Screen 2 Excel File.xls | 🗑 Remove | ⊕ Upload | 📂 Browse ... |

*Figure 7: Input and Output file upload options*

4. Once the files are uploaded, the matches found by the program are displayed in a table. The table contains a checkbox which enables you to select or deselect the given match, the input column which is the column number indicator in the excel file (A, B, C, ...), the input header which is the column name of the input header, the corresponding matched output column (A, B, C, ...) and the output header which are from the uploaded output file.

5. You can click on the checkboxes of each match to select or deselect the matches.

6. You can also add new matches by clicking on the "Add More" button. After clicking on this button, three dropdown boxes are displayed: the first one contains the list of input headers, the second one contains the list of intermediate headers and the last one contains the list of output headers. You can choose any input header, corresponding intermediate header and the output header to match with that input header. If you want to remove this additional match, click on

Choose Matches for Anatrace_MCSG1_Formulations-Excel.xlsx and MD1-02_Structure_Screen_2_Excel_File.xls

|   | Input Column | Input Header | Output Column | Output Header |
|---|---|---|---|---|
| ☑ | Select All | | | |
| ☑ | B | Well | A | Tube # |
| ☑ | C | [Salt] | B | Conc1 |
| ☑ | D | [Salt] units | C | Units1 |
| ☑ | E | Salt | D | Salt 1 |
| ☑ | F | [Buffer] | K | Conc4 |
| ☑ | G | [Buffer] units | L | Units4 |
| ☑ | H | Buffer | M | Buffer4 |
| ☑ | J | pH | N | pH |
| ☑ | K | [PPT1] | O | Conc5 |
| ☑ | L | [PPT1] Units | P | Units5 |
| ☑ | M | Precipitant 1 | Q | Precipitant5 |
| ☑ | N | [PPT2] | R | Conc6 |
| ☑ | O | [PPT2] Units | S | Units6 |
| ☑ | P | Precipitant 2 | T | Precipitant6 |

Add More

Accept

*Figure 8: Input-to-output matches*

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the "Remove" button beside the match. Click on the "Add More" button add another match.



*Figure 9: Option to add more matches*

7.  There is an additional header named "Other" in the intermediate headers list. This option can be chosen if the user does not know which intermediate header to select or for additional columns not present in the intermediate headers.
8.  Once you are done selecting the matches, click on the "Accept" button.
9.  The next page shown is to add display names for unseen chemicals. If no unseen chemicals are found in the input screen file, then this page is skipped (see step 13).



*Figure 10: Choose display names for unseen*

10. This page displays the IUPAC name for a chemical and a dropdown box with the list of possible names for the chemical (default selection is the IUPAC name itself). For each chemical, choose a display name from the dropdown list. If you wish to add a name not mentioned in the dropdown

list, choose the "Other" option in the dropdown menu and a text box will appear. Type the display name for the chemical in the text box.

11. There is a "Skip now" checkbox to the right of every dropdown button which is checked by default in order to skip entering display names for selected chemicals. If it is checked, the display name for that chemical is not saved to database and will be asked next time. The checkbox is automatically unchecked when the selection of the dropdown changes and can also be changed manually by clicking on it.

12. After choosing display names for all chemicals, click on the "Submit" button.

12. Then the output file will be written to the output folder inside the ScreenMatcher folder. You can also use the "Download file" button to directly download the output file to a desired location. You can continue to convert another file by go to this home page http:// http://datamedia.cs.uah.edu/screenmatcher and repeating above steps.

** If using web browser backward navigation, make sure that you refresh the ScreenMatcher home page.



**Output file is ready:** [Download File]

Matches for Anatrace_MCSG1_Formulations-Excel and MD1-02_Structure_Screen_2_Excel_File

| Input Column | Input Header | Output Column | Output Header |
|---|---|---|---|
| B | Well | A | Tube # |
| C | [Salt] | B | Conc1 |
| D | [Salt] units | C | Units1 |
| E | Salt | D | Salt 1 |
| F | [Buffer] | K | Conc4 |
| G | [Buffer] units | L | Units4 |
| H | Buffer | M | Buffer4 |
| I | Titrated With | G | Salt 2 |
| J | pH | N | pH |
| K | [PPT1] | O | Conc5 |
| L | [PPT1] Units | P | Units5 |
| M | Precipitant 1 | Q | Precipitant5 |
| N | [PPT2] | R | Conc6 |
| O | [PPT2] Units | S | Units6 |
| P | Precipitant 2 | T | Precipitant6 |

*Figure 11: Final matches and output file download page*



| | A | B | C | D | E | F | G | H | I | J | K | L | M | N | O | P | Q | R | S | T |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | Tube # | Conc1 | Units1 | Salt 1 | Conc2 | Units2 | Salt 2 | Conc3 | Units3 | Salt 3 | Conc4 | Units4 | Buffer4 | pH | Conc5 | Units5 | Precipitant5 | Conc6 | Units6 | Precipitant6 |
| 2 | a1 | | | | | | sodium hydroxide | | | | 0.1 | m | hepes | 7.5 | 20 | % (w/v) | peg 8000 | | | |
| 3 | a2 | | | | | | sodium hydroxide | | | | 0.1 | m | ches | 9.5 | 30 | % (w/v) | peg 3000 | | | |
| 4 | a3 | 0.2 | m | sodium chloride | | | | | | | 0.1 | m | na2hpo4/kh2po4 | 6.2 | 10 | % (w/v) | peg 8000 | | | |
| 5 | a4 | 0.2 | m | magnesium chloride | | | hydrogen chloride | | | | 0.1 | m | tris | 7 | 2.5 | m | sodium chloride | | | |
| 6 | a5 | 0.2 | m | sodium chloride | | | acetic acid | | | | 0.1 | m | sodium acetate | 4.5 | 1.26 | m | ammonium sulfate | | | |
| 7 | a6 | 0.2 | m | ammonium sulfate | | | hydrogen chloride | | | | 0.1 | m | bis-tris | 5.5 | 25 | % (w/v) | peg 3350 | | | |
| 8 | a7 | 0.2 | m | magnesium chloride | | | hydrogen chloride | | | | 0.1 | m | bis-tris | 5.5 | 25 | % (w/v) | peg 3350 | | | |
| 9 | a8 | | | | | | hydrogen chloride | | | | 0.1 | m | tris | 7 | 20 | % (w/v) | peg mme 2000 | | | |
| 10 | a9 | 0.2 | m | magnesium chloride | | | sodium hydroxide | | | | 0.1 | m | hepes | 7.5 | 25 | % (w/v) | peg 3350 | | | |
| 11 | a10 | 0.2 | m | calcium chloride | | | sodium hydroxide | | | | 0.1 | m | hepes | 7.5 | 28 | % (v/v) | ppg p400 | | | |
| 12 | a11 | 0.2 | m | magnesium chloride | | | sodium hydroxide | | | | 0.1 | m | mes | 6.5 | 10 | % (w/v) | peg 4000 | | | |
| 13 | a12 | 0.2 | m | calcium chloride | | | hydrogen chloride | | | | 0.1 | m | tris | 8.5 | 20 | % (w/v) | peg 4000 | | | |
| 14 | b1 | 0.6 | m | sodium chloride | | | sodium hydroxide | | | | 0.1 | m | mes | 6.5 | 20 | % (w/v) | peg 4000 | | | |
| 15 | b2 | 0.2 | m | sodium chloride | | | hydrogen chloride | | | | 0.1 | m | bis-tris | 5.5 | 25 | % (w/v) | peg 3350 | | | |
| 16 | b3 | 0.2 | m | ammonium acetate | | | hydrogen chloride | | | | 0.1 | m | bis-tris | 5.5 | 25 | % (w/v) | peg 3350 | | | |
| 17 | b4 | 0.2 | m | magnesium chloride | | | hydrogen chloride | | | | 0.1 | m | bis-tris | 6.5 | 25 | % (w/v) | peg 3350 | | | |
| 18 | b5 | 0.2 | m | magnesium chloride | | | hydrogen chloride | | | | 0.1 | m | tris | 8.5 | 25 | % (w/v) | peg 3350 | | | |
| 19 | b6 | 0.2 | m | calcium diacetate hydrate | | | sodium hydroxide | | | | 0.1 | m | mes | 6 | 25 | % (w/v) | peg 8000 | | | |
| 20 | b7 | 0.17 | m | ammonium acetate | | | hydrogen chloride | | | | 0.085 | m | sodium citrate | 5.6 | 25.5 | % (w/v) | peg 4000 | 15 | % (v/v) | glycerol |
| 21 | b8 | 0.17 | m | sodium acetate | | | hydrogen chloride | | | | 0.085 | m | tris | 8.5 | 25.5 | % (w/v) | peg 4000 | 15 | % (v/v) | glycerol |
| 22 | b9 | 0.2 | m | magnesium chloride | | | | | | | | | | | 20 | % (w/v) | peg 3350 | | | |
| 23 | b10 | 0.16 | m | magnesium chloride | | | hydrogen chloride | | | | 0.08 | m | tris | 8.5 | 24 | % (w/v) | peg 4000 | 20 | % (v/v) | glycerol |
| 24 | b11 | 0.2 | m | magnesium chloride | | | hydrogen chloride | | | | 0.1 | m | tris | 8.5 | 20 | % (w/v) | peg 8000 | | | |
| 25 | b12 | | | | | | hydrogen chloride | | | | 0.1 | m | bis-tris | 6.5 | 28 | % (w/v) | peg mme 2000 | | | |

*Figure 12: Example of output file of Anatrace MCSG file in MD1-02 screen format*