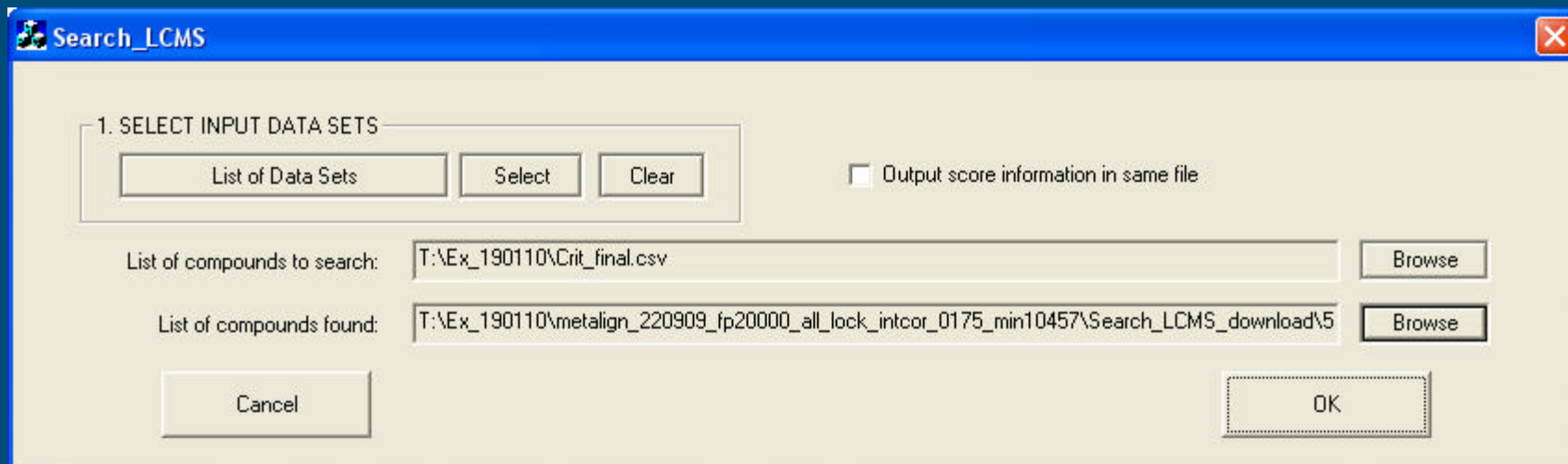


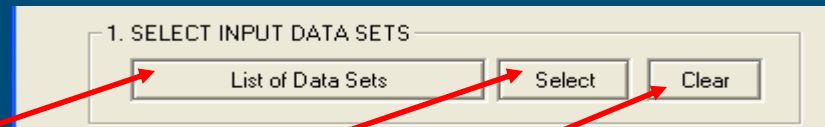
Search_LCMS: searches metAlign-reduced data

Metalign creates “redms_acc” files in a subfolder called “baseline” in a “Final_results_folder”. These small files (100-1000x reduced) contain all the information of accurate mass LC-MS files.

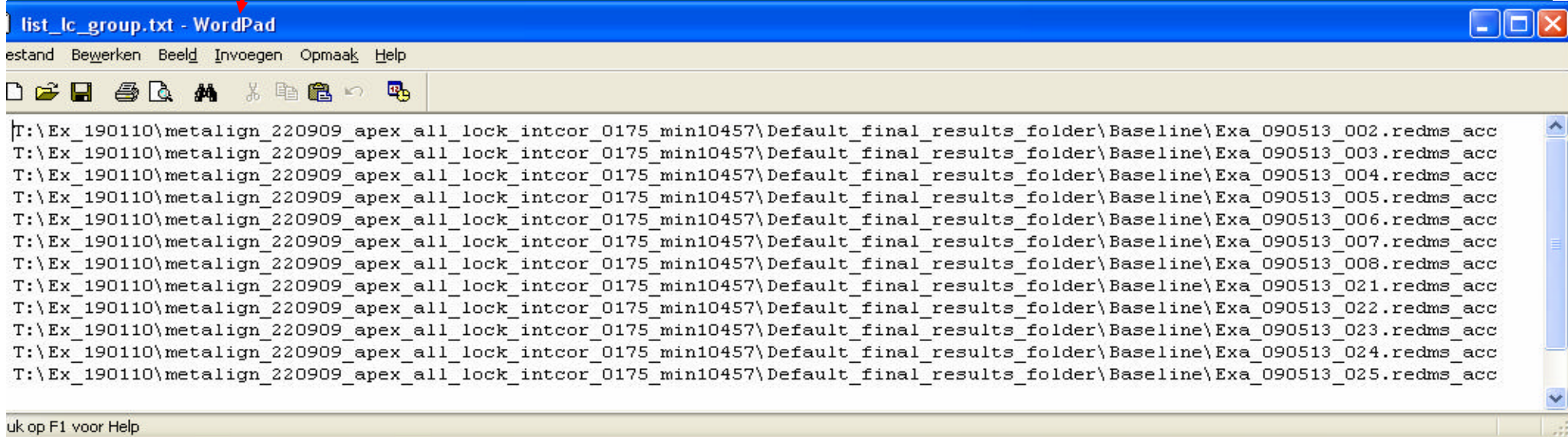
Search_LCMS is an ultra-fast program for searching “redms_acc” files.



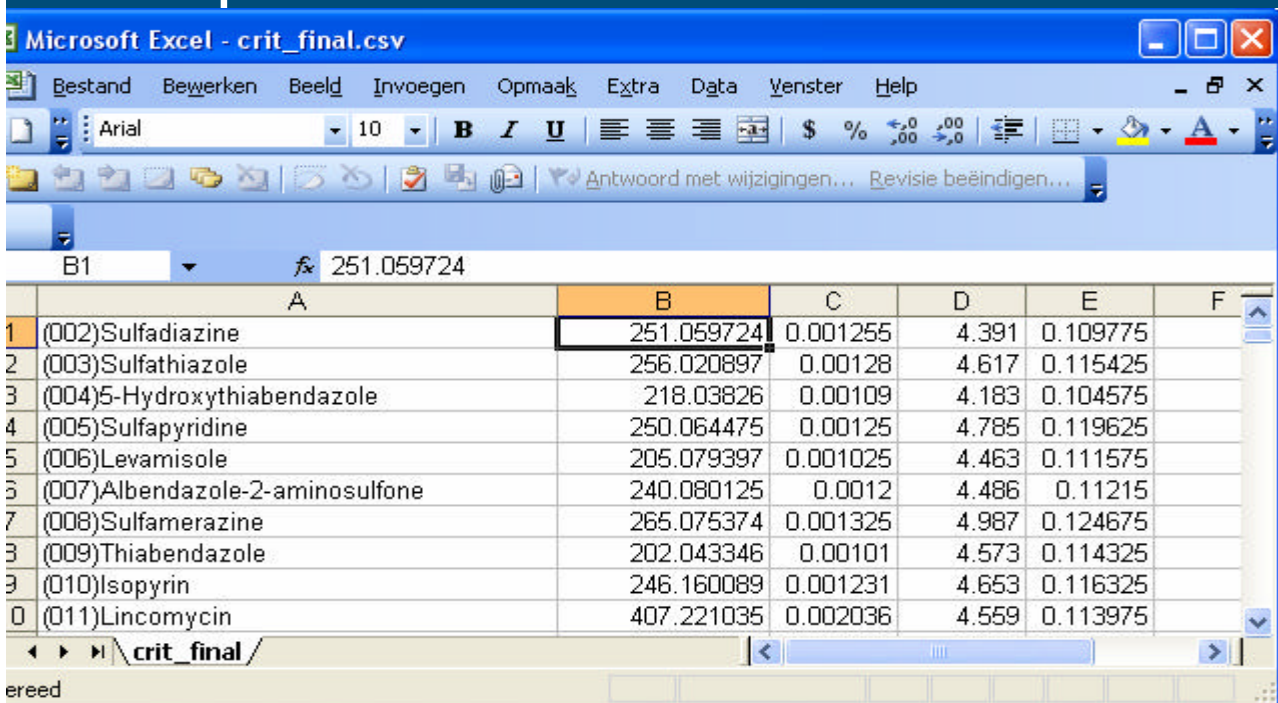
Search_LCMS: defining which redms_acc files



- “List of Data Sets” button: The list of “redms_acc” files selected for searching can be viewed here using wordpad.
- “Select” button (files appear in “selected box”): this module is described in “metalign_manual.ppt” slide 6 and is used to select “redms_acc” files.
- “Clear” button resets the selection



Search LCMS: defining search criteria in Excel: multiple compounds with retentions



Microsoft Excel - crit_final.csv

Bestand Bewerken Beeld Invoegen Opmaak Extra Data Venster Help

Arial 10 B I U

Antwoord met wijzigingen... Revisie beëindigen...

B1 251.059724

	A	B	C	D	E	F
1	(002)Sulfadiazine	251.059724	0.001255	4.391	0.109775	
2	(003)Sulfathiazole	256.020897	0.00128	4.617	0.115425	
3	(004)5-Hydroxythiabendazole	218.03826	0.00109	4.183	0.104575	
4	(005)Sulfapyridine	250.064475	0.00125	4.785	0.119625	
5	(006)Levamisole	205.079397	0.001025	4.463	0.111575	
6	(007)Albendazole-2-aminosulfone	240.080125	0.0012	4.486	0.11215	
7	(008)Sulfamerazine	265.075374	0.001325	4.987	0.124675	
8	(009)Thiabendazole	202.043346	0.00101	4.573	0.114325	
9	(010)Isopyrin	246.160089	0.001231	4.653	0.116325	
10	(011)Lincomycin	407.221035	0.002036	4.559	0.113975	

crit_final/

ereed

Note: this file is stored as a csv file in Excel!

First column may be used to name a compound.

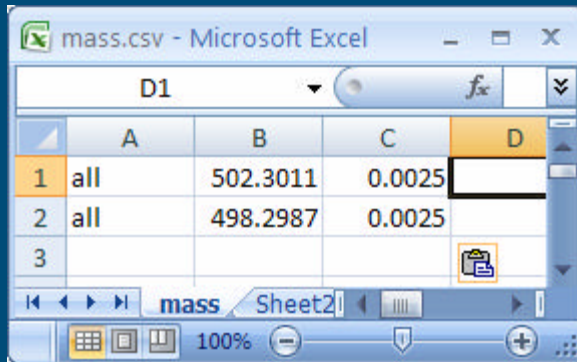
Second column contains the mass to search.

Third column contains “delta mass”: mass window = mass +/- delta mass.

Fourth column contains the retention time in minutes.

Fifth column contains “delta retention” in minutes: retention window = retention +/- delta retention.

Search LCMS: defining search criteria in Excel: all defined masses through out the chromatogram

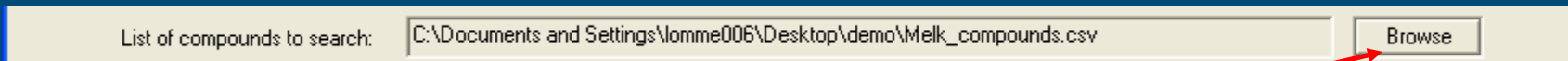


	A	B	C
1	all	502.3011	0.0025
2	all	498.2987	0.0025
3			

Note: this file is stored as a csv file in Excel!

- First column must be used to for the term “all”. This determines the search mode.
- Second column contains the mass to search.
- Third column contains “delta mass”: mass window = mass +/- delta mass.

Search_LCMS: selecting the search criteria csv file

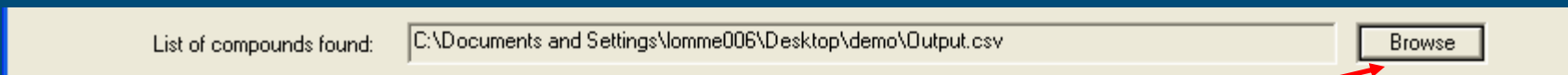


- “Browse” button: this is used to select the search criteria csv file (see previous slide).

Note: this part is described in “metalign_manual.ppt” slide 6 and is used to select “csv” files.



Search_LCMS: selecting the output csv file

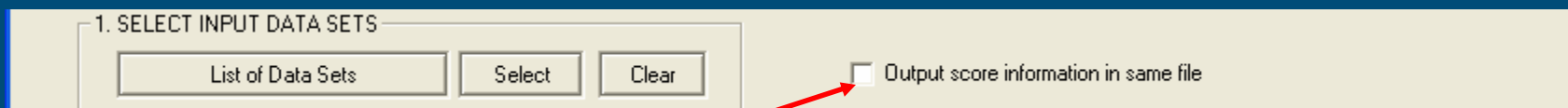


- “Browse” button: this is used to select the output csv file (see previous slide).

Note: this part is described in “metalign_manual.ppt” slide 6 and is used to select “csv” files.



Search_LCMS: Output description



Pressing the “OK” button generates output:

- If “Output score information in same file” is unchecked, all information is stored in separate files: output.csv (ampl/intensity), output_mass.csv (mass), output_noise.csv (noise), output_ppm.csv (ppm error), output_ret.csv (retention), output_scan.csv (scan).
- If “Output score information in same file” is checked, all information (but not all) is stored in one file: output.csv
- Using a search file as described in slide 4 (“all”) option ignores the option “Output score information in same file” and generates one output file: output.csv

ote: output.csv (“Output score information in same file” = unchecked) is compatible with GM2MS (see documentation of metalign -> Additional_metalign_related_tools.ppt); conversion to MS format is possible