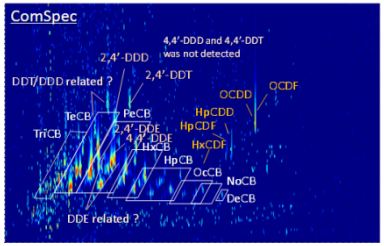

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Operation manual of GUI-based ComSpec

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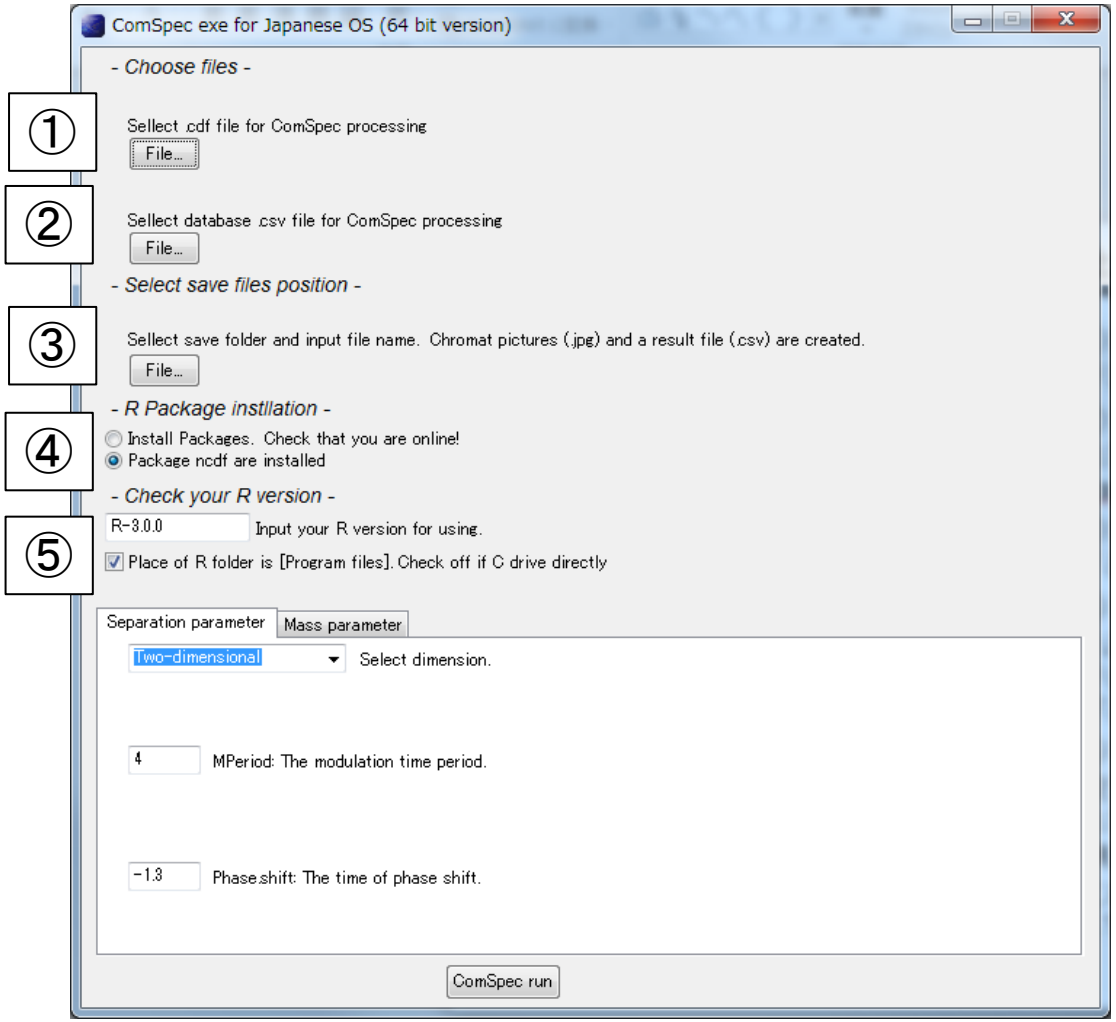
Hardware Requirements for ComSpec.exe

- OS: Windows 7 (English Edition)
- More than 10 GB RAM is recommended for large data.
- Installation of Statistical software “R” is required. Freely downloadable from the site below.
- http://cran.md.tsukuba.ac.jp/bin/windows/base/
- netCDF data from Agilent, Waters, JEOL (GC and LC) have been confirmed to work.
- Don’t touch the computer keyboard during first minute, because this tool automatically types the required information instead of you. Please save and close important files before starting the calculation (Don’t place the important files at “My documents”, for safety.).
- Data for a demonstration is available via the following link (Japanese site).
- http://www.nies.go.jp/analysis/member.html#downloads

How to Operate 1



①Choose the data that you want to analyze (.cdf).

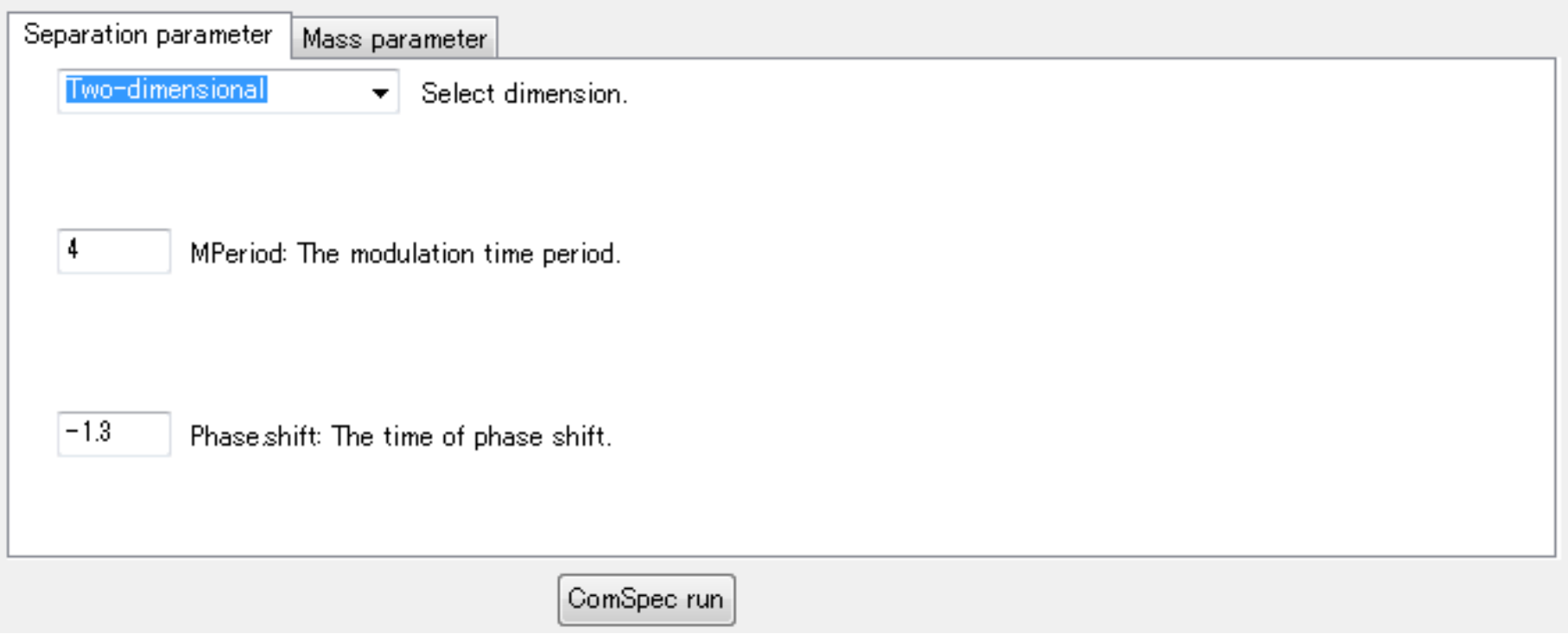
②Choose the database file that includes your target compounds (.csv).

③Set the output folder and file name.

④In the first time, installation of program packages are needed. Choose the upper one.

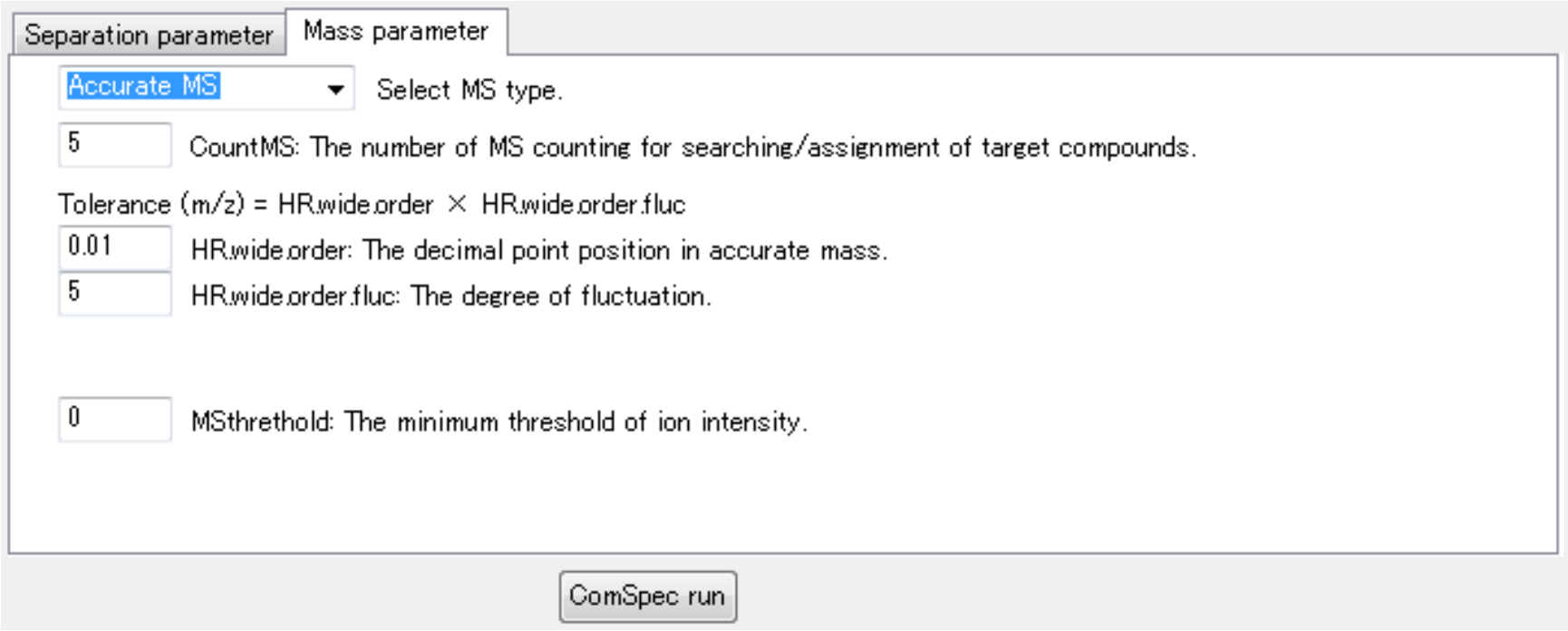
⑤Set file path for calling “R”. You need to recognize where and which version of “R” is installed on your computer. Located at C drive directly or “Program Files”?

How to Operate 2



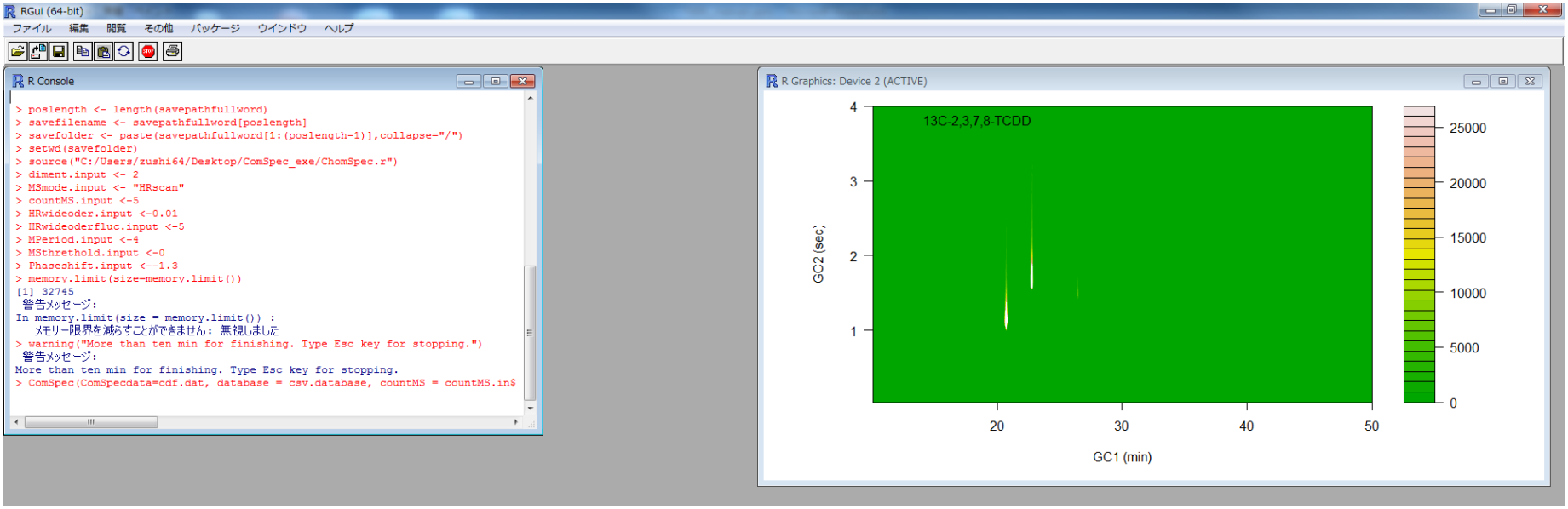
- Set the parameter of separation in your data. 1D or 2D data?
- Enter parameters of ”Mperiod” and “Phase.shift” in the box.
- In the case of 1D, ”Mperiod” and “Phase.shift” is not used, so you don’t need to change the default setting.

How to Operate 3



- Set the parameter of Mass in your collected data.
- Accurate or Nominal MS?
- If you chose “Accurate MS”, information on mass accuracy (Tolerance) is needed. Input the parameter according to the screen displays.
- In the case of nominal MS, “HRwide.order” and “Hrwide.order.fluc” is not used, so you don’t need to change the default setting.
- After setting all the parameters, click the “ComSpec run” button.

Screenshot of the Tool Execution



- If all the parameters are correctly set, “R” will boot up and your setting will be loaded. Don’t touch to keyboard during this process.
- If all the code is loaded in “R”, target search will be started.
- Generally, it takes 30 seconds for 1 list search. If you have 100 lists, it takes around 50 minutes for all the calculation.
- After the calculation, you can find the output files, such as XXX.jpeg and XXX.csv (the file names depends on your setting), in the save folder you set.

Output (.csv) file

Sum of Ion intensity (see *Analytica Chimica Acta*, 778, (17), 54–62, 2013. for the detail)

	A	B	C
1		Chemical Group	Total Intensity
2	1	13C-1,3,6,8-TC	755951.2686
3	2	13C-2,3,7,8-TC	675241.3295
4	3	13C-2,3,7,8-TC	845765.7558
5	4	13C-1,2,3,7,8-P	1067394.943
6	5	13C-2,3,4,7,8-P	1139565.646
7	6	13C-1,2,3,7,8-P	413155.4418
8	7	13C-1,2,3,4,7,8-	2400718.739
9	8	13C-1,2,3,6,7,8-	2420457.081
10	9	13C-2,3,4,6,7,8-	1902501.398
11	10	13C-1,2,3,4,7,8-	1412971.102
12	11	13C-1,2,3,6,7,8-	1192387.261
13	12	13C-1,2,3,7,8,9-	1210614.606
14	13	13C-1,2,3,7,8,9-	2181478.082
15	14	13C-1,2,3,4,6,7,	794531.7906
16	15	13C-1,2,3,4,6,7,	322024.2945
17	16	13C-1,2,3,4,7,8,	959849.9805
18	17	13C-OCDD	463800.7483
19	18	13C-OCDF	516117.5448
20	19	2,3,7,8-TCDF	3425557.111
21	20	2,3,7,8-TCDD	2557332.038
22	21	1,2,3,7,8-PeCDI	6406933.802
23	22	2,3,4,7,8-PeCDI	6240099.218
24	23	1,2,3,7,8-PeCDI	2075728.916
25	24	1,2,3,4,7,8-HxC	9563031.872
26	25	1,2,3,6,7,8-HxC	9594927.783
27	26	2,3,4,6,7,8-HxC	9451968.644

Chemical Group name
(Individual names are presented here just for this demonstration)

- The listed name and its ion quantified value is reported (Sum of ion intensity is calculated and adjusted by several ions which you set, and finally the intensity of the first ion in the database is returned.). The intensity ratio of native to IS whose combination is set in database is also calculated.

About the Database

Chemical Group name
(Individual names are presented here just for this demonstration)

MS fragment

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V
1	BlobID	Compound Abriviation	Group Nam	Rtcorrect	Internal Standard	Peak I	Peak II	IS_Native_ref									MS1	MS2	MS3	MS4	MS5	MS6
2	-1	13C-2,3,7,8-TCDF	PCDD	1	1	22.24	0.834	0									317.95283	315.94825	319.93246	318.92842	316.93021	321.92677
3																	15.265677	12.887926	9.9872899	4.4107563	2.5250874	2.3886481
4		13C-1,3,6,8-TCDD	PCDD	0	1	20.63	0.001	1									333.9487	331.94479	335.93219	267.97001	269.96701	204.00319
5																	12.049672	10.114774	8.0782124	6.1127712	5.8802501	2.8517746
6	2	13C-2,3,7,8-TCDF	PCDD	4	1	22.24	0.834	2									317.95283	315.94825	319.93246	251.9708	253.96762	182.03453
7																	15.265677	12.887926	9.9872899	3.685348	3.5346513	3.128246
40	19	2,3,7,8-TCDF	PCDD	0	0	22.24	0.834	2									305.89596	303.89921	307.89436	240.9406	242.93661	171.00252
41																	22.536902	17.63751	10.841941	4.0036323	3.9958859	3.8846943
42	20	2,3,7,8-TCDD	PCDD	0	0	22.77	0.278	3									321.89055	319.89321	323.88787	256.93147	258.92932	193.97054

- Calculation starts from the top of this list. The same process is repeated over other chemical list in this order.
- Information of a compound is stored in 2 rows. The first row is for m/z. The second row is for relative intensity (total of these values should be 100%).
- Only columns “B” and “Q -” are used for the calculation.
- Cells from “I” to “P” are available for remarks, in case you want to use them.

Precautions

-About the source file

- Keep the position of source file “ComSpec.r” with the same position of ComSpec.exe file.

-If the software freeze, exit from it by clicking icon in bottom light.

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