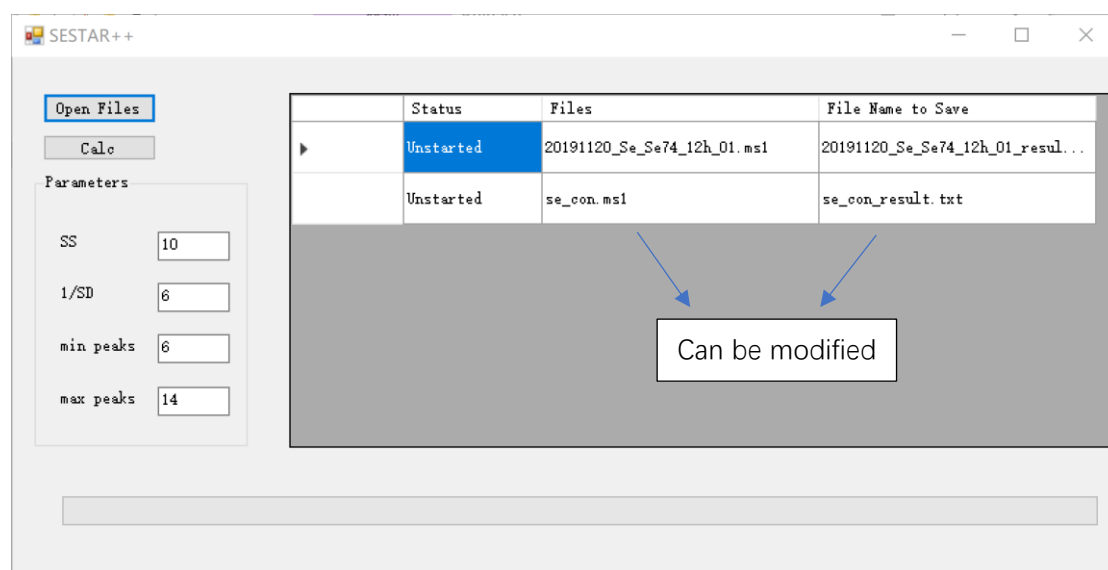


How to get results:



1. Open SESTAR_GUI.exe
2. Click "Open Files" button, and select *.ms1 file(s) to be processed.
3. Rows can be deleted if wrong files are selected. File name to open/save can be modified in the sheet (Make sure the file name is available).
4. Set appropriate parameters. Recommended parameters are shown below. Of course, you can set your own parameters within the limits.

	Limit	Loose	Strict
SS	>0 (decimal)	15	10
1/SD	>=0 (decimal)	4	6
Min peaks	>0 (integer)	5	6
Max peaks	<=14 (integer)	14	14

5. Click "Calc" and be patient. ;-)

How to interpret results:

1. Open the result file (Excel is recommended). Every row represents a potential candidate and sorted by the scan number. Candidates with lower "SS.Se" and higher "SD.Se" are more likely containing selenium. More specifically, "SS.Se" describes the similarity between observed envelope and theoretical envelope with selenium, while "SD.Se" represents the uniqueness of the similarity to only the selenium-containing envelope but not the proteogenic counterpart.

1	retention.time	charge	mass	mz.max	mz	intensity	calc.se.dist	SS.Se	SD.Se	scan.No
2	11.24251	3	1314.585	439.2022	438.5335	435258.1	110.1546033	4.590526	10.55418	2079
3	12.16925	3	1318.637	440.5528	439.8796	410833.6	410.1543758	7.620584	6.830223	2247
4	12.28828	3	1176.567	393.1962	392.1923	5322.5	1210.0709472	9.335705	7.006888	2268
5	12.29907	2	1193.579	597.7969	596.2889	27757.6	410.0706470	7.674311	8.515975	2270
6	12.34555	2	1193.579	597.7969	596.2895	26725.7	410.0706470	7.228959	8.463049	2278
7	12.35095	2	1193.577	597.7959	596.2897	23733	4150.0706470	7.46265	8.49293	2279
8	12.39205	2	1028.452	515.2335	513.23	5112927.7	810.0551555	9.616364	8.140587	2286
9	12.83844	2	1309.533	655.774	654.275	612056.2	310.0692453	5.140306	11.72349	2366
10	12.93456	3	1549.612	517.5445	516.5476	7134.9	1310.0658811	9.956669	6.742762	2383
11	12.93456	3	1352.593	451.8717	450.8684	7795.4	1010.0685342	8.257457	6.838684	2383
12	12.98619	2	1309.534	655.7745	654.2745	11701.9	310.0692453	8.957527	7.277471	2392
13	12.99698	2	1309.532	655.7734	654.2723	7525.2	3810.0692453	9.275255	6.951735	2394
14	13.0433	2	1309.534	655.7744	654.275	619131.9	3510.0692453	7.206026	9.068492	2402
15	13.0487	2	1309.534	655.7743	654.2738	114040.4	210.0692453	6.532532	10.09055	2403
16	13.0541	2	1309.534	655.7744	654.7759	30803.8	110.1546033	6.29019	8.860815	2404
17	13.10034	2	970.4252	486.2199	484.7144	7389.9	1710.0733561	7.265663	8.783823	2412
18	13.11113	2	1309.534	655.7743	654.7766	40996.8	210.1546033	7.859925	6.342012	2414
19	13.2139	1	459.2053	460.2126	456.1952	20960.6	610.0753723	8.769439	9.026943	2432
20	13.38722	2	1155.494	578.7544	577.2546	8922.9	1510.0713081	5.024858	11.95937	2463
21	13.46586	3	1306.606	436.5425	435.5381	4402.5	2510.0692453	7.627582	8.560473	2477
22	13.47125	2	845.4412	423.7279	422.2202	5329.2	1310.0747626	8.176275	8.601869	2478
23	13.57338	2	1121.475	561.7449	560.2337	6811	27090.0717399	6.180169	10.69635	2496
24	13.60135	3	1306.606	436.5427	435.8746	37523.5	210.1546033	5.800836	8.378604	2501

- Sort all rows by "mass" so that candidates with the same mass will get closer. More candidates with the same mass mean this peptide is continuously observed in a series of full mass scans, so it's less likely a false positive result. If candidates with different charges but the same mass are observed in the same full mass scan, they are very likely true positive results. You can return to raw data to check if selenium-containing isotopic pattern can be observed.

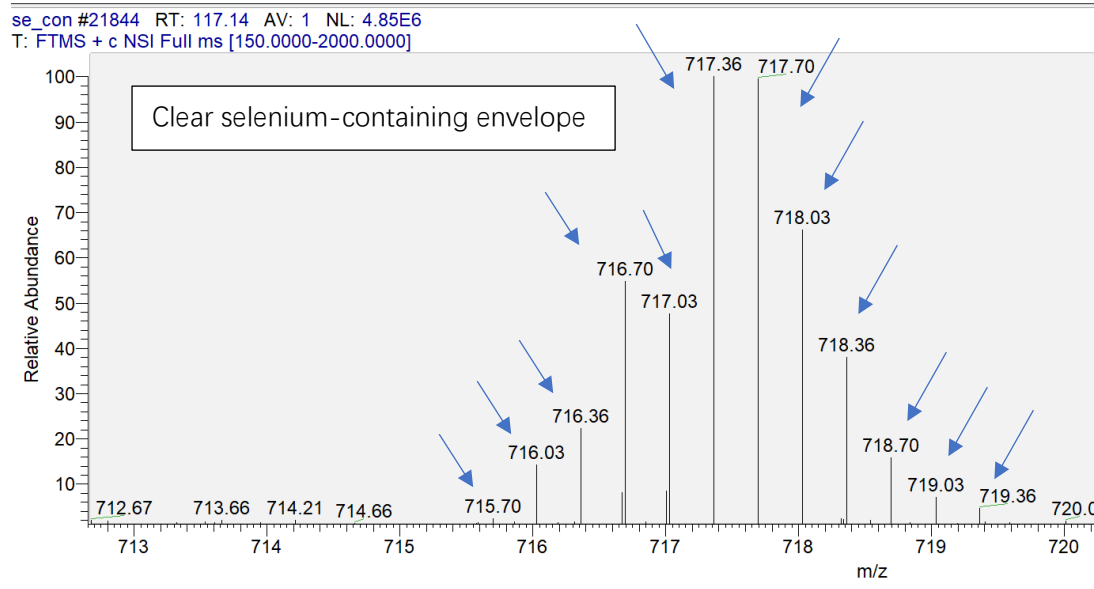
retention.time	charge	mass	mz.max	mz	intensity	calc.se.dist	SS.Se	SD.Se	scan.No
81.66495	3	2146.025	716.3488	715.0048	56629.4	910.0304566	9.2262	6.562177	15181
129.0720	2	2146.025	1074.263	1072.2689	39694.9	410.0304566	8.853435	6.968285	24068
40.41	2	2146.025	716.6448	715.312	7100241.8	100.0565750	9.598548	6.968285	24068
102.2	2	2146.025	716.6864	715.3505	43812.8	610.0565750	7.290624	7.290624	24068
136.5094	3	2147.101	716.7075	715.3679	40083.8	410.0565750	7.519456	7.519456	24068
81.86465	3	2148.961				65750	7.211394	7.211394	24068
90.6931	3	2149.01				04525	9.538708	7.692692	16878
117.0363	3	2149.056				30867	9.306893	8.726464	21825
117.4368	2	2149.062				04525	5.327948	12.90084	21900
117.4695	3	2149.063	717.3615	715.3637	153038.5	10.0027127	3.287068	25.70907	21906
117.4695	2	2149.063	1075.539	1073.5411	500429.4	10.0304525	2.717363	24.98102	21906
117.4917	2	2149.063	1075.539	1073.5403	371858.5	10.0304525	5.844284	11.48299	21910
117.1366	3	2149.064	717.3618	715.7004	118243.9	10.0030867	2.886962	27.04818	21844
117.4585	3	2149.064	717.3618	715.3646	194847.4	10.0027127	3.673641	22.98031	21904
117.7767	3	2149.064	717.3618	715.3635	67189.4	810.0027127	7.633131	10.90461	21964
117.3939	2	2149.064	1075.539	1073.5396	385997	610.0304525	3.828047	17.8153	21892
117.4585	2	2149.064	1075.539	1073.5398	257875.9	10.0304525	5.707217	12.04724	21904
117.6073	3	2149.064	717.3619	715.3649	143601.3	10.0027127	2.986863	27.91717	21932
117.4917	3	2149.064	717.362	715.363	786004.1	110.0027127	3.501021	24.11319	21910
117.718	3	2149.064	717.362	716.03	71276025.7	10.0304525	5.166993	13.32841	21953
117.2274	3	2149.064	717.3621	715.6972	83275.9	110.0030867	3.34273	22.91156	21861
117.6392	3	2149.065	717.3622	715.3655	62409.1	810.0027127	4.396876	19.32281	21938
118.7539	3	2149.065	717.3624	716.0311	77667.1	410.0304525	7.9816	8.313242	22145
117.3725	2	2149.066	1075.541	1073.0469	88686.6	310.0030867	5.800325	13.16986	21888
117.6073	2	2149.066	1075.541	1073.5425	149046.9	10.0304525	4.109724	16.48263	21932
117.2432	3	2149.067	717.3628	715.3644	120420.7	10.0027127	1.509193	55.5786	21864
117.6229	3	2149.067	717.3628	716.0303	1235300.9	10.0304525	4.16201	16.20053	21935
117.1258	3	2149.067	717.3629	715.7006	62246	3640.0030867	4.324173	18.37106	21842
117.2274	2	2149.067	1075.541	1073.5442	208204.8	10.0304525	5.387958	12.26863	21861
117.19	3	2149.067	717.363	715.3653	138058.5				854
117.2754	3	2149.067	717.363	715.3646	87667.178				870

Different charge

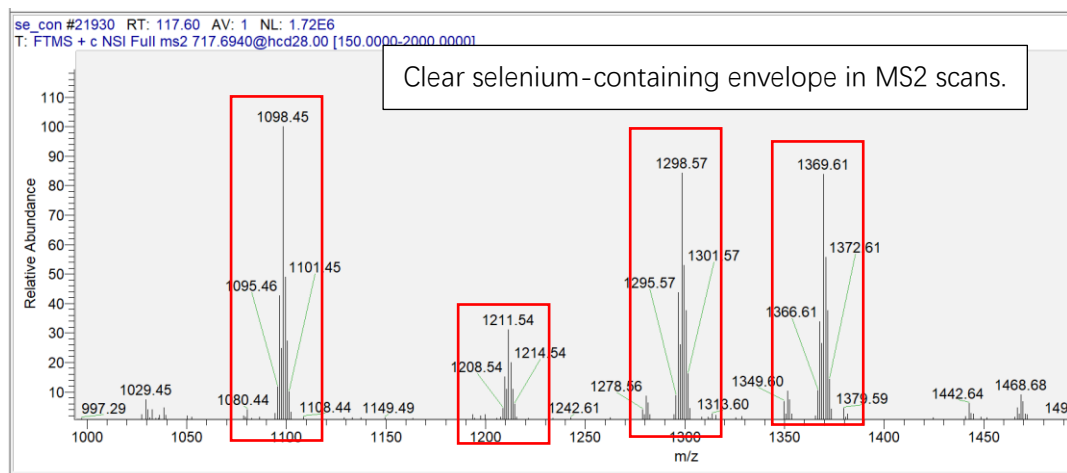
Continuous scans suggest they may be the same peptides

Many candidates with the same mass

Low SS.Se and high SD.Se



3. Check the MS2 scans of candidates selected from Step 2. If selenium-encoded isotopic patterns are also observed, record them as candidates with very high possibility to be selenium-containing peptides.



4. Database searching or *de novo* sequencing or other further processing. (The above example is GPX1 according to the database searching results)