Electronic Supplementary Material (ESI) for Analytical Methods.

Super-resolution Raman imaging towards improved visualisation of nanoplastics

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Supporting Information

Contents

1. Figure S1 / Table S1: More information for Figures 2-3

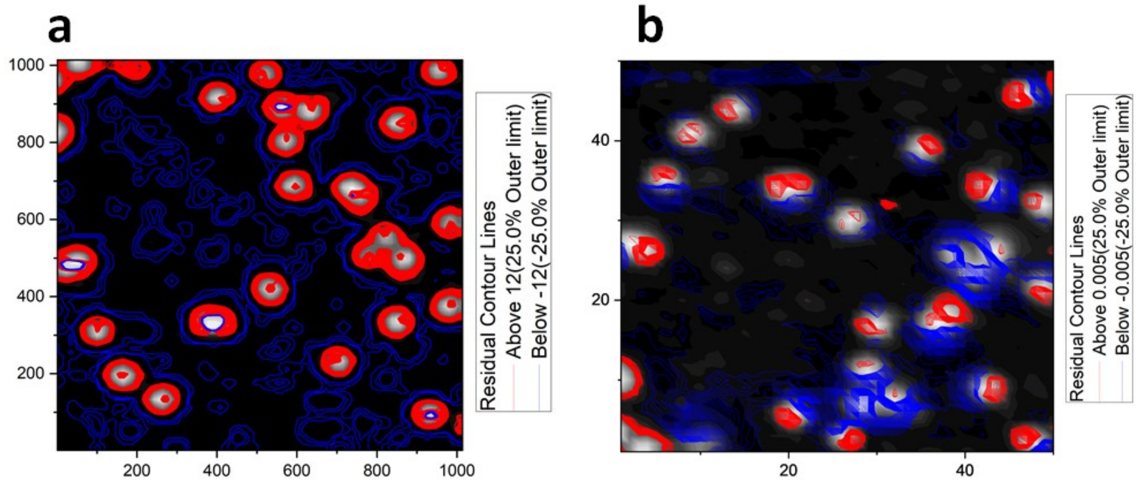

Figure S1. Fitting residues for Figures 2-3. (a) is for Figure 2 (without PCA) while (b) is for Figure 3 (with PCA).

Figure S1 shows the fitting residues. In (a), while the strong signals are paid more attention, the weak signal has a very limited contribution, which needs more research. Particularly, once these weak signal can be confirmed as the nanoplastics, the fitting should covered them as well to re-construct the image, as shown in Figure 3 and in (b). Note the fitting in (a) starts up from the Raman intensity image with a pixel of 1024 × 1024, while (b) starts up from the loading coefficient of an array of 50 × 50.

Table S1. Parameters Summary for the fitting peaks (all data for the x × y axis of 1014× 1014, after removing boundary from 1024× 1024 of the image with size of 10 μm × 10 μm). The highlight (in yellow) marks the peaks for Figures 2(i, j).

	z0		A		xc		w1		yc		w2		FWHMx		FWHMy	
	Value	Standard Error	Value	Standard Error	Value	Standard Error	Value	Standard Error	Value	Standard Error	Value	Standard Error	Value	Standard Error	Value	Standard Error
Peak1(Sheet1)	18.38568	--	235.61432	--	50	--	11	--	482	--	7.68987	--	25.90302	0	18.10825	0
Peak2(Sheet1)	18.38568	--	235.61432	--	61	--	10.09146	--	482	--	7.10049	--	23.76356	0	16.72038	0
Peak3(Sheet1)	18.38568	--	235.61432	--	39	--	11	--	482	--	7.35467	--	25.90302	0	17.31892	0
Peak4(Sheet1)	18.38568	--	235.61432	--	28	--	12.76591	--	482	--	7.35095	--	30.06143	0	17.31016	0
Peak5(Sheet1)	18.38568	--	235.61432	--	738	--	5.68465	--	666	--	4.794	--	13.38633	0	11.28901	0

Peak6(Sheet1)	18.38568	--	235.61432	--	410	--	5.68465	--	338	--	7.68987	--	13.38633	0	18.10825	0
Peak7(Sheet1)	18.38568	--	235.61432	--	403	--	9	--	338	--	9.5642	--	21.19338	0	22.52198	0
Peak8(Sheet1)	18.38568	--	235.61432	--	392	--	11	--	338	--	7.35467	--	25.90302	0	17.31892	0
Peak9(Sheet1)	18.38568	--	235.61432	--	756	--	17.47346	--	666	--	7.35095	--	41.14685	0	17.31016	0
Peak10(Sheet1)	18.38568	--	235.61432	--	390	--	12.76591	--	318	--	4.21869	--	30.06143	0	9.93425	0
Peak11(Sheet1)	18.38568	--	235.61432	--	389	--	17.27454	--	325	--	12.76591	--	40.67842	0	30.06143	0
Peak12(Sheet1)	18.38568	--	235.61432	--	370	--	7.35467	--	338	--	8.18595	--	17.31892	0	19.27645	0
Peak13(Sheet1)	18.38568	--	235.61432	--	381	--	11	--	338	--	10.06029	--	25.90302	0	23.69018	0
Peak14(Sheet1)	18.38568	--	235.61432	--	861	--	8.97483	--	502	--	6.36249	--	21.1341	0	14.98252	0
Peak15(Sheet1)	18.38568	--	234.61432	--	164	--	12.66748	--	195	--	6.8439	--	29.82962	0	16.11616	0
Peak16(Sheet1)	18.38568	--	234.61432	--	267	--	9.20559	--	134	--	8.00881	--	21.67751	0	18.8593	0
Peak17(Sheet1)	18.38568	--	234.61432	--	860	--	10.57892	--	338	--	6.8439	--	24.91145	0	16.11616	0
Peak18(Sheet1)	18.38568	--	234.61432	--	942	--	8.4191	--	93	--	6.50569	--	19.82546	0	15.31974	0
Peak19(Sheet1)	18.38568	--	234.61432	--	554	--	6.34886	--	891	--	7.04577	--	14.95042	0	16.59152	0
Peak20(Sheet1)	18.38568	--	234.61432	--	22	--	10.34517	--	482	--	9.20559	--	24.36102	0	21.67751	0
Peak21(Sheet1)	18.38568	--	234.61432	--	934	--	9.5	--	93	--	6.50569	--	22.37079	0	15.31974	0
Peak22(Sheet1)	18.38568	--	234.61432	--	923	--	7.97825	--	93	--	6.50569	--	18.78735	0	15.31974	0
Peak23(Sheet1)	18.38568	--	234.61432	--	561	--	12.73874	--	891	--	6.25576	--	29.99743	0	14.7312	0
Peak24(Sheet1)	18.38568	--	233.61432	--	574	--	6.3352	--	809	--	7.32319	--	14.91825	0	17.24478	0
Peak25(Sheet1)	18.38568	--	233.61432	--	572	--	14.50212	--	891	--	7.29021	--	34.14989	0	17.16714	0
Peak26(Sheet1)	18.38568	--	233.61432	--	594	--	9.26266	--	687	--	6.4917	--	21.8119	0	15.28678	0
Peak27(Sheet1)	18.38568	--	233.61432	--	635	--	7.9409	--	890	--	11.37935	--	18.69939	0	26.79631	0
Peak28(Sheet1)	18.38568	--	233.61432	--	983	--	9.3218	--	379	--	6.82919	--	21.95117	0	16.08152	0
Peak29(Sheet1)	18.38568	--	233.61432	--	533	--	9.99679	--	420	--	8.823	--	23.54064	0	20.77657	0
Peak30(Sheet1)	18.38568	--	231.61432	--	859	--	12.76346	--	850	--	7.70846	--	30.05565	0	18.15204	0
Peak31(Sheet1)	18.38568	--	228.61432	--	410	--	9.08654	--	912	--	5.49379	--	21.39717	0	12.9369	0
Peak32(Sheet1)	18.38568	--	224.61432	--	103	--	6.21088	--	317	--	10.60366	--	14.62551	0	24.96971	0
Peak33(Sheet1)	18.38568	--	210.61432	--	697	--	14.51675	--	236	--	5.92406	--	34.18433	0	13.95009	0
Peak34(Sheet1)	18.38568	--	204.61432	--	963	--	8.59387	--	993	--	8.36909	--	20.23702	0	19.70769	0
Peak35(Sheet1)	18.38568	--	193.61432	--	820	--	6.21228	--	563	--	9.83776	--	14.6288	0	23.16616	0
Peak36(Sheet1)	18.38568	--	173.61432	--	984	--	6.59385	--	584	--	9.95422	--	15.52733	0	23.44039	0
Peak37(Sheet1)	18.38568	--	164.61432	--	513	--	7.98692	--	973	--	9.69053	--	18.80777	0	22.81944	0
Peak38(Sheet1)	18.38568	--	151.61432	--	779	--	6.15823	--	502	--	9.29644	--	14.50152	0	21.89144	0
Peak39(Sheet1)	18.38568	--	84.61432	--	185	--	11.45345	--	994	--	5.38304	--	26.97082	0	12.67609	0
Peak40(Sheet1)	18.38568	--	54.61432	--	1004	--	3.50268	--	72	--	5.21737	--	8.24818	0	12.28597	0
Peak41(Sheet1)	18.38568	--	12.61432	--	686	--	2.89694	--	912	--	2.89694	--	6.82176	0	6.82176	0
Peak42(Sheet1)	18.38568	--	6.61432	--	901	--	3.08455	--	563	--	3.08455	--	7.26357	0	7.26357	0
Peak43(Sheet1)	18.38568	--	4.61432	--	226	--	1.68456	--	543	--	2.46706	--	3.96683	0	5.80949	0
Peak44(Sheet1)	18.38568	--	4.61432	--	243	--	1.68456	--	543	--	1.68456	--	3.96683	0	3.96683	0
Peak45(Sheet1)	18.38568	--	4.61432	--	233	--	1.68456	--	544	--	2.49907	--	3.96683	0	5.88486	0
Peak46(Sheet1)	18.38568	--	3.61432	--	185	--	1.46287	--	51	--	1.98225	--	3.44481	0	4.66784	0

2. Figure S2 / Table S2: More information for Figure 3

2.1. PCA analysis parameters for Figure 3

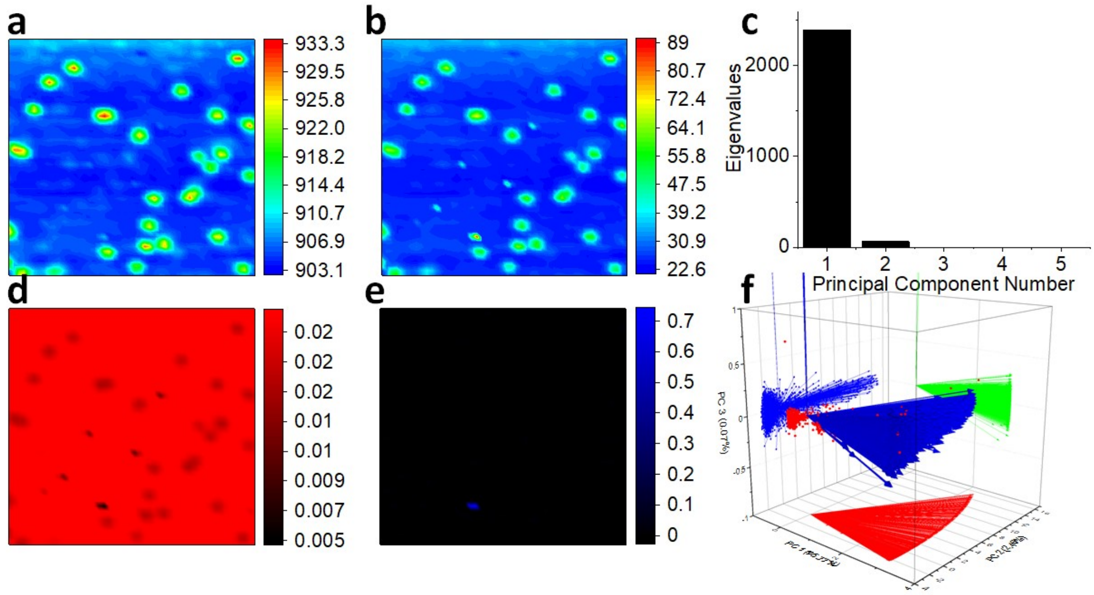

Figure S2. PCA analysis on the raw data in Figure 2, including the mapped mean (a), standard variation (b), scree plot (c), mapped coefficients of PC1 (d) and PC3 (e), loading plot (f).

Figure S2 shows the PCA analysis parameters for Figure 3. The mapped mean can tell us where the main signal (or main variance) are collected. The mapped variation reminds us where the PCA calculation is not so confident and we should be cautious to draw the conclusion. Scree plot indicates the main variance of PCA analysis is taken in PC1 and PC2.

The mapped coefficients of PC1 and PC3 can support the assignment of PC1 to background, and PC3 to noise, such as cosmic ray from the detector. The loading plot implied that most of the PCs are independent from each other.

2.2. Fitting parameters for Figure 3

Table S2. Parameters Summary for the fitting peaks (all data for the x × y axis of 50 × 50, for the image with size of 10 μm × 10 μm).

	z0		A		xc		w1		yc		w2		FWHMx		FWHMy		Volume
	Value	Standard Error	Value	Standard Error	Value	Standard Error	Value	Standard Error	Value	Standard Error	Value	Standard Error	Value	Standard Error	Value	Standard Error	Value
Peak1(PC2)	-0.00483	--	0.08847	--	20	--	1.72769	--	34	--	1.34432	--	4.06839	0	3.16564	0	1.29111
Peak2(PC2)	-0.00483	--	0.08837	--	37	--	1.5442	--	17	--	1.58568	--	3.63632	0	3.73399	0	1.35954
Peak3(PC2)	-0.00483	--	0.08789	--	2	--	1.93986	--	27	--	1.33572	--	4.56801	0	3.14537	0	1.43083
Peak4(PC2)	-0.00483	--	0.08757	--	43	--	1.58337	--	26	--	1.64652	--	3.72855	0	3.87726	0	1.43444
Peak5(PC2)	-0.00483	--	0.08631	--	28	--	1.82243	--	7	--	1.29551	--	4.2915	0	3.0507	0	1.28036
Peak6(PC2)	-0.00483	--	0.08527	--	49	--	1.25536	--	32	--	1.30274	--	2.95614	0	3.06773	0	0.87621
Peak7(PC2)	-0.00483	--	0.08468	--	9	--	1.37387	--	41	--	1.22444	--	3.23522	0	2.88334	0	0.89502
Peak8(PC2)	-0.00483	--	0.08412	--	30	--	1.16125	--	17	--	1.29341	--	2.73454	0	3.04576	0	0.79387
Peak9(PC2)	-0.00483	--	0.08381	--	27	--	1.36013	--	30	--	1.31291	--	3.20285	0	3.09166	0	0.94036
Peak10(PC2)	-0.00483	--	0.08265	--	43	--	1.33339	--	34	--	1.30912	--	3.1399	0	3.08275	0	0.9065
Peak11(PC2)	-0.00483	--	0.08225	--	29	--	1.4725	--	11	--	1.24779	--	3.46746	0	2.93831	0	0.94955
Peak12(PC2)	-0.00483	--	0.08204	--	41	--	1.42554	--	23	--	1.63661	--	3.35688	0	3.85392	0	1.20258
Peak13(PC2)	-0.00483	--	0.08167	--	47	--	1.31558	--	46	--	0.97728	--	3.09795	0	2.30132	0	0.65973
Peak14(PC2)	-0.00483	--	0.0809	--	6	--	1.30259	--	35	--	1.26196	--	3.06737	0	2.97169	0	0.83561
Peak15(PC2)	-0.00483	--	0.08072	--	32	--	1.78627	--	7	--	1.35577	--	4.20634	0	3.1926	0	1.2282
Peak16(PC2)	-0.00483	--	0.08046	--	14	--	1.30012	--	44	--	1.16984	--	3.06155	0	2.75477	0	0.76886
Peak17(PC2)	-0.00483	--	0.08017	--	42	--	1.4463	--	9	--	1.22376	--	3.40579	0	2.88174	0	0.8916
Peak18(PC2)	-0.00483	--	0.07976	--	48	--	1.18141	--	2	--	1.26634	--	2.782	0	2.98201	0	0.74974
Peak19(PC2)	-0.00483	--	0.07913	--	21	--	1.31643	--	6	--	1.09707	--	3.09997	0	2.5834	0	0.71807
Peak20(PC2)	-0.00483	--	0.07901	--	35	--	1.24467	--	39	--	1.23578	--	2.93097	0	2.91005	0	0.76357
Peak21(PC2)	-0.00483	--	0.07322	--	49	--	1.58042	--	22	--	1.3003	--	3.72159	0	3.06197	0	0.9454
Peak22(PC2)	-0.00483	--	0.07212	--	26	--	1.05846	--	3	--	1.16269	--	2.49248	0	2.73793	0	0.55768
Peak23(PC2)	-0.00483	--	0.07104	--	39	--	1.45564	--	26	--	1.51739	--	3.42776	0	3.57319	0	0.98585
Peak24(PC2)	-0.00483	--	0.04454	--	10	--	1.8007	--	2	--	2.44108	--	4.24033	0	5.74831	0	1.23026
Peak25(PC2)	-0.00483	--	0.01197	--	13	--	1.08461	--	24	--	0.7814	--	2.55407	0	1.84005	0	0.06375
Peak26(PC2)	-0.00483	--	0.00717	--	11	--	1.38732	--	35	--	2.24834	--	3.2669	0	5.29444	0	0.14059
Peak27(PC2)	-0.00483	--	0.00591	--	10	--	14	--	48	--	0.5	--	32.96748	0	1.17741	0	0.26002
Peak28(PC2)	-0.00483	--	0.00574	--	20	--	0.97835	--	25	--	0.75286	--	2.30383	0	1.77284	0	0.02654
Peak29(PC2)	-0.00483	--	0.00402	--	33	--	1.00291	--	44	--	2.74131	--	2.36168	0	6.45529	0	0.0695
Peak30(PC2)	-0.00483	--	0.00399	--	8	--	16.5	--	7	--	3.26426	--	38.85453	0	7.68675	0	1.34868
Peak31(PC2)	-0.00483	--	0.00384	--	19	--	0.99048	--	18	--	1.5	--	2.3324	0	3.53223	0	0.03586
Peak32(PC2)	-0.00483	--	0.0035	--	41	--	2.41875	--	41	--	2.12025	--	5.69571	0	4.99281	0	0.11284
Peak33(PC2)	-0.00483	--	-0.00214	--	20	--	10	--	45	--	6.28993	--	23.5482	0	14.81164	0	-0.845
Peak34(PC2)	-0.00483	--	0.0021	--	12	--	1.01556	--	12	--	1.52402	--	2.39147	0	3.58878	0	0.02042
Peak35(PC2)	-0.00483	--	0.00205	--	23	--	11	--	49	--	1	--	25.90302	0	2.35482	0	0.14172
Peak36(PC2)	-0.00483	--	0.00203	--	12	--	2.30303	--	20	--	1	--	5.42323	0	2.35482	0	0.02944
Peak37(PC2)	-0.00483	--	-0.00192	--	27	--	13.5	--	45	--	0.5	--	31.79007	0	1.17741	0	-0.08122
Peak38(PC2)	-0.00483	--	-0.00172	--	30	--	12	--	35	--	2	--	28.25784	0	4.70964	0	-0.25974
Peak39(PC2)	-0.00483	--	0.00167	--	34	--	2.71388	--	48	--	0.44996	--	6.39071	0	1.05957	0	0.01284
Peak40(PC2)	-0.00483	--	-0.00162	--	20	--	16	--	41	--	2.79409	--	37.67712	0	6.57958	0	-0.45376
Peak41(PC2)	-0.00483	--	--	--	--	--	0	--	--	--	0	--	0	0	0	0	--

Peak42(PC2)	-0.00483	--	--	--	--	--	0	--	--	--	0	--	0	0	0	0	--

3. Figure S3 / Table S3: More information for Figures 4-5

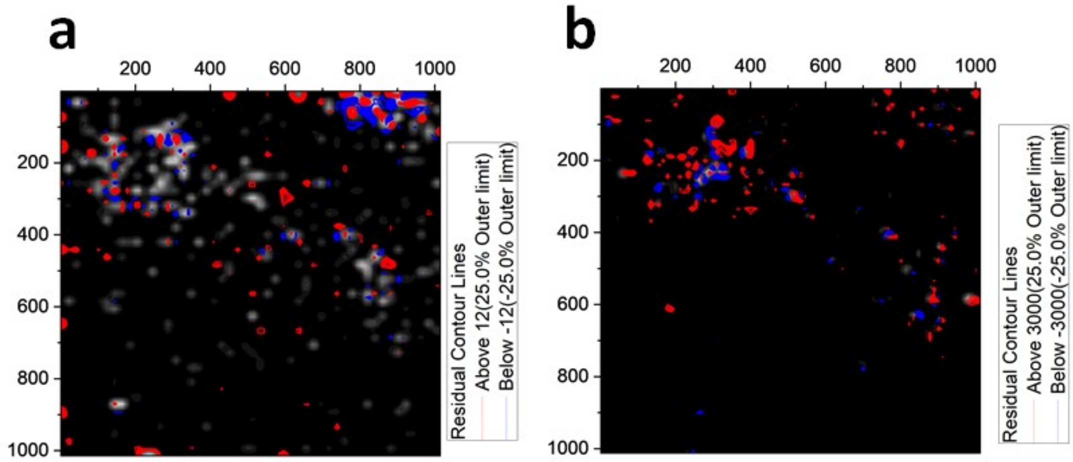

Figure S3. Fitting residue for Figures 4-5. (a) is for Figure 4 while (b) for Figure 5.

Due to the weak signal and the computation complexity, there are lots of spots that are not picked up for fitting in (a). This limit also corresponds with the image resolution issue discussed in the main manuscript. That is, we must balance among the high resolution imaging (to capture nanoplastics down to < 100 nm), the scanning duration, the signal intensity and the computation capacity etc.

This fitting residue in (b) looks better than (a), because the logic-based algorithm has filtered lots of noise towards fitting.

Table S3. Parameters Summary for the fitting peaks (all data for the x × y axis of 1014× 1014, after removing boundary from 1024× 1024 of the image with size of 2 μm × 2 μm). The highlight (in yellow) marks the peaks for Figures 3(i, j).

	z0		A		xc		w1		yc		w2		FWHMx		FWHMy	FWHMy
	Value	Standard Error	Value	Standard Error	Value	Standard Error	Value	Standard Error	Value	Standard Error	Value	Standard Error	Value	Standard Error	Value	Standard Error
Peak1([??]!VM1)	0.84463	--	77.79409	0.62121	296.46938	0.19256	14.36979	0.1826	275.75727	0.0884	9.71212	0.09074	33.83826	0.43	22.87029	0.21368
Peak2([??]!VM1)	0.84463	--	201.02913	2.58203	306.43863	0.21125	9.38256	0.13613	194.27497	0.05477	9.98574	0.05362	22.09423	0.32057	23.51462	0.12627
Peak3([??]!VM1)	0.84463	--	200.03753	2.92847	287.10754	0.21358	8.94307	0.11009	194.59261	0.03931	9.03248	0.04273	21.05932	0.25925	21.26987	0.10063
Peak4([??]!VM1)	0.84463	--	201.62757	2.50669	164.73751	0.19285	9.16101	0.10814	870.76214	0.03712	9.05154	0.03699	21.57254	0.25465	21.31474	0.08711
Peak5([??]!VM1)	0.84463	--	209.41154	2.2406	144.58551	0.19875	9.5833	0.11113	871.04875	0.03468	9.05904	0.03455	22.56694	0.26169	21.33242	0.08135
Peak6([??]!VM1)	0.84463	--	0.79294	0.28061	721.36923	--	1.2202E96	2740473.47828	870.97107	0.34095	0.64918	0.24376	2.87336E96	0	1.5287	0.57402
Peak7([??]!VM1)	0.84463	--	227.66274	0.51665	253.11224	0.06906	21.91385	0.0861	113.38731	0.02517	9.65815	0.02614	51.60318	0.20276	22.7432	0.06155
Peak8([??]!VM1)	0.84463	--	185.8738	0.407	294.081	0.07374	24.0278	0.06376	140.14811	0.05072	14.73689	0.04891	56.58113	0.15015	34.70272	0.11518
Peak9([??]!VM1)	0.84463	--	198.89545	0.80012	348.54575	0.05517	10.75032	0.05261	153.70381	0.03698	7.74636	0.03678	25.31506	0.12389	18.24129	0.08661
Peak10([??]!VM1)	0.84463	--	189.27429	0.55638	787.43412	0.03842	18.56866	0.04165	1	0.42264	49.21518	0.26506	43.72584	0.09809	115.8929	0.62417
Peak11([??]!VM1)	0.84463	--	206.89683	0.64419	267.74252	0.05944	9.85968	0.05047	257.16921	0.09251	16.29867	0.07206	23.21776	0.11885	38.38044	0.1697
Peak12([??]!VM1)	0.84463	--	230.19136	0.44594	908.92817	0.03839	18.94744	0.04178	24.43127	0.02939	15.10098	0.0339	44.61781	0.0984	35.56009	0.07983
Peak13([??]!VM1)	0.84463	--	207.64874	0.88151	902.69392	0.03874	8.38493	0.03865	72.06712	0.03616	7.7834	0.03673	19.745	0.09102	18.3285	0.08649
Peak14([??]!VM1)	0.84463	--	217.52066	0.76874	801.13168	0.06284	10.33094	0.05643	481.59121	0.03326	9.00434	0.03404	24.32751	0.13289	21.20361	0.08016
Peak15([??]!VM1)	0.84463	--	211.28785	0.58974	323.48852	0.06709	14.3226	0.05432	170.68749	0.06021	12.35155	0.05818	33.72714	0.12793	29.08568	0.137
Peak16([??]!VM1)	0.84463	--	212.13551	0.65419	46.26689	0.04065	13.13297	0.04053	31.16459	0.02763	8.8785	0.02787	30.92578	0.09545	20.90726	0.06562
Peak17([??]!VM1)	0.84463	--	227.0082	0.48885	134.11733	0.04443	20.40636	0.04487	135.10125	0.02517	10.53494	0.02702	48.05331	0.10565	24.80789	0.06362
Peak18([??]!VM1)	0.84463	--	238.61509	0.47604	837.60499	0.02921	12.52272	0.02972	35.45709	0.03763	18.48326	0.04153	29.48874	0.06999	43.52475	0.09779
Peak19([??]!VM1)	0.84463	--	231.62447	0.49625	871.81463	0.03911	15.5829	0.0412	87.08117	0.03078	13.56722	0.02973	36.69492	0.09703	31.94837	0.07001
Peak20([??]!VM1)	0.84463	--	208.19887	0.70558	203.44462	0.03909	11.32235	0.04044	277.05234	0.03103	9.00253	0.03156	26.66209	0.09522	21.19933	0.07433
Peak21([??]!VM1)	0.84463	--	241.92333	0.61352	328.44086	0.02345	8.93462	0.02353	224.03346	0.04485	15.58428	0.04783	21.03942	0.05542	36.69818	0.11263
Peak22([??]!VM1)	0.84463	--	217.55524	0.61021	146.68063	0.03943	13.41466	0.04109	172.32238	0.03469	10.81283	0.03837	31.58911	0.09675	25.46226	0.09036
Peak23([??]!VM1)	0.84463	--	225.79125	0.61896	335.67001	0.04141	14.79251	0.04194	338.37644	0.02509	8.96501	0.0255	34.8337	0.09875	21.11099	0.06004
Peak24([??]!VM1)	0.84463	--	194.83997	0.56467	842.21813	0.04287	12.48565	0.04247	459.92604	0.03924	12.822	0.03877	29.40146	0.1	30.1935	0.09131
Peak25([??]!VM1)	0.84463	--	207.35605	0.59941	513.28763	0.06201	16.01098	0.05429	297.35153	0.03091	8.96203	0.02901	37.70297	0.12784	21.10396	0.06832
Peak26([??]!VM1)	0.84463	--	215.13781	0.78955	21.19747	0.03301	8.99398	0.03367	215.51049	0.03276	8.95805	0.03288	21.17921	0.07928	21.0946	0.07742
Peak27([??]!VM1)	0.84463	--	214.24278	0.77834	246.75905	0.03445	9.19847	0.03463	215.76532	0.03362	9.07305	0.0342	21.66073	0.08154	21.3654	0.08053
Peak28([??]!VM1)	0.84463	--	162.83867	1.39701	246.91474	0.04502	7.95292	0.05828	321.69739	0.08003	13.00036	0.0877	18.72769	0.13723	30.61352	0.20651
Peak29([??]!VM1)	0.84463	--	187.64088	0.48933	523.02378	0.05851	21.95706	0.06356	236.57401	0.0257	9.93551	0.02593	51.70492	0.14968	23.39634	0.06106
Peak30([??]!VM1)	0.84463	--	175.96494	0.58123	621.58315	0.04791	14.52107	0.04813	400.28179	0.03375	10.21828	0.03399	34.19452	0.11333	24.0622	0.08003
Peak31([??]!VM1)	0.84463	--	181.58767	0.7887	512.73692	0.0388	8.93304	0.03882	625.1489	0.03883	8.93931	0.03884	21.0357	0.09141	21.05047	0.09147
Peak32([??]!VM1)	0.84463	--	172.28654	0.67171	104.83077	0.14414	15.07768	0.1518	194.16146	0.04132	9.68015	0.03826	35.50522	0.35746	22.79502	0.09009
Peak33([??]!VM1)	0.84463	--	174.44708	0.80098	861.4564	0.06487	9.47709	0.05985	584.41706	0.04476	8.93093	0.04488	22.31685	0.14094	21.03073	0.10567
Peak34([??]!VM1)	0.84463	--	186.26434	0.68464	820.00223	0.03478	8.42879	0.03275	498.81048	0.11238	16.88241	0.09068	19.84828	0.07713	39.75504	0.21354
Peak35([??]!VM1)	0.84463	--	154.1	0.61164	143.3926	0.03534	9.79841	0.03966	263.49944	0.08704	21.69103	0.10031	23.0735	0.09338	51.07847	0.23621
Peak36([??]!VM1)	0.84463	--	173.9849	0.75016	492.22917	0.03876	9.00624	0.03879	196.01932	0.04254	9.84334	0.04288	21.20809	0.09133	23.1793	0.10098
Peak37([??]!VM1)	0.84463	--	163.78687	0.71953	62.93611	0.06268	10.3121	0.06589	193.92829	0.04631	10.01151	0.0461	24.28313	0.15517	23.57531	0.10855
Peak38([??]!VM1)	0.84463	--	167.02102	0.73176	534.65756	0.0486	10.23429	0.04787	317.35617	0.05548	9.41495	0.05386	24.0999	0.11272	22.1705	0.12683
Peak39([??]!VM1)	0.84463	--	171.14086	0.6034	820.89905	0.03564	10.01959	0.03727	569.47082	0.04946	13.97462	0.05031	23.59434	0.08777	32.90773	0.11848
Peak40([??]!VM1)	0.84463	--	164.23297	0.52247	985.40149	0.03733	11.60571	0.03893	113.88232	0.05115	16.13007	0.05224	27.32936	0.09168	37.98341	0.12302

4. Table S4: More information for Figure 5

Table S4. Parameters Summary for the fitting peaks (all data for the x × y axis of 1014× 1014, after removing boundary from 1024× 1024 of the image with size of 2 μm × 2 μm)

	z0		A		xc		w1		yc		w2		FWHMx		FWHMy	FWHMy
	Value	Standard Error	Value	Standard Error	Value	Standard Error	Value	Standard Error	Value	Standard Error	Value	Standard Error	Value	Standard Error	Value	Standard Error
Peak1(Sheet1)	179.15111	0.44221	40357.6704	62.57202	297	0.04098	6.97647	0.03663	233	0.06213	9.26526	0.05799	16.42833	0.08626	21.81801	0.13655
Peak2(Sheet1)	179.15111	0.44221	48004.42713	--	284	0.03499	7.79692	0.03124	234	0.04032	8.84231	0.04087	18.36035	0.07357	20.82205	0.09624
Peak3(Sheet1)	179.15111	0.44221	53585.94757	218.217	265	0.03005	8.91765	0.03319	256	0.03037	8.65814	0.03449	20.99945	0.07815	20.38836	0.08123
Peak4(Sheet1)	179.15111	0.44221	52584.25652	197.52463	982	0.02832	9.14197	0.03075	584	0.02721	8.47805	0.02791	21.52769	0.07241	19.96428	0.06573
Peak5(Sheet1)	179.15111	0.44221	34137.22974	253.99116	313	0.0788	7.64874	0.07398	216	0.16574	7.69689	0.14638	18.01142	0.1742	18.1248	0.34469
Peak6(Sheet1)	179.15111	0.44221	41580.3121	208.92286	326	0.05331	9.83388	0.05099	233	0.0566	9.96324	0.05025	23.15702	0.12008	23.46164	0.11832
Peak7(Sheet1)	179.15111	0.44221	37393.91565	219.55028	384	0.03841	8.85732	0.04225	175	0.0381	8.78351	0.04187	20.85738	0.09949	20.68358	0.0986
Peak8(Sheet1)	179.15111	0.44221	43212.45222	185.93137	838	0.03962	7.9299	0.03841	625	0.02764	5.52834	0.02674	18.67349	0.09045	13.01824	0.06296
Peak9(Sheet1)	179.15111	0.44221	33765.2093	209.61686	60	0.04404	9.87183	0.04886	236	0.04076	9.13833	0.04538	23.24639	0.11505	21.51912	0.10686
Peak10(Sheet1)	179.15111	0.44221	33691.32798	243.90051	900	0.0361	4.14215	0.0387	441	0.06688	7.00466	0.0607	9.75401	0.09112	16.49472	0.14295
Peak11(Sheet1)	179.15111	0.44221	30392.26752	194.10424	511	0.05197	10.75636	0.05811	297	0.04459	9.07727	0.04872	25.32929	0.13684	21.37533	0.11473
Peak12(Sheet1)	179.15111	0.44221	24770.4869	219.29031	306	0.05609	6.49132	0.05887	182	0.06989	8.18059	0.07742	15.28589	0.13864	19.26383	0.1823
Peak13(Sheet1)	179.15111	0.44221	39587.81232	347.2641	204	0.03831	2.55242	0.03979	31	0.04266	3.4361	0.04744	6.01049	0.09369	8.0914	0.11172
Peak14(Sheet1)	179.15111	0.44221	15606.17611	230.53184	195	0.05661	4.81149	0.06231	277	0.17682	13.02471	0.19817	11.33019	0.14673	30.67084	0.46665
Peak15(Sheet1)	179.15111	0.44221	27777.95144	223.75394	758	0.08737	9.18206	0.06369	399	0.09369	7.78662	0.07297	21.62209	0.14999	18.3361	0.17183
Peak16(Sheet1)	179.15111	0.44221	20370.6793	239.73185	446	0.03224	2.42634	0.03278	277	0.15904	11.63123	0.15039	5.71359	0.07718	27.38945	0.35414
Peak17(Sheet1)	179.15111	0.44221	16462.1786	376.67008	347	0.08801	4.98262	0.09521	163	0.08688	4.92513	0.09403	11.73317	0.22421	11.59778	0.22143
Peak18(Sheet1)	179.15111	0.44221	22253.97114	195.32811	879	0.0724	8.70123	0.07439	584	0.06499	7.62383	0.06387	20.48982	0.17517	17.95274	0.15041
Peak19(Sheet1)	179.15111	0.44221	31847.16419	1428.32374	244	0.05463	0.87806	0.04981	206	0.05217	0.53769	0.02873	2.06767	0.11729	1.26615	0.06766
Peak20(Sheet1)	179.15111	0.44221	23557.19107	206.37754	429	0.08599	6.93947	0.08253	236	0.0435	3.53738	0.04173	16.3412	0.19435	8.32989	0.09826
Peak21(Sheet1)	179.15111	0.44221	15816.3192	401.51925	489	0.18228	4.60541	0.16613	277	0.04546	1.15825	0.04233	10.84491	0.39121	2.72747	0.09967
Peak22(Sheet1)	179.15111	0.44221	25545.20819	211.52851	818	0.0589	9.33909	0.06408	502	0.0533	8.44061	0.0579	21.99188	0.15089	19.87611	0.13635
Peak23(Sheet1)	179.15111	0.44221	16813.53053	907627.50944	305	2332840.76556	1.40229E-4	3361106.67002	99	--	0.02228	--	3.30214E-4	7914801.36304	0.05245	--
Peak24(Sheet1)	179.15111	0.44221	17463.03996	172.81691	255	0.06751	7.2623	0.06902	220	0.11656	11.6294	0.11941	17.10142	0.16254	27.38514	0.28119
Peak25(Sheet1)	179.15111	0.44221	15020.2359	188.00367	293	0.17654	4.29804	0.17776	208	0.10296	2.47505	0.10355	10.12112	0.41859	5.8283	0.24385
Peak26(Sheet1)	179.15111	0.44221	1254.72558	796.61913	252	--	1.71966	1.62999	228	0.75612	1.72175	1.7321	4.04949	3.83832	4.05441	4.07878
Peak27(Sheet1)	179.15111	0.44221	17199.32266	198.75532	125	0.09003	9.36792	0.09897	181	0.07895	8.40373	0.08391	22.05977	0.23305	19.78928	0.1976
Peak28(Sheet1)	179.15111	0.44221	16157.67471	2156.42749	308	0.12902	0.53645	0.07211	93	3653.8226	0.18693	--	1.26324	0.16981	0.4402	--
Peak29(Sheet1)	179.15111	0.44221	16608.39143	154.86754	293	0.07615	9.60852	0.08582	133	0.13743	19.13259	0.13634	22.62635	0.20209	45.05381	0.32105
Peak30(Sheet1)	179.15111	0.44221	16732.29254	250.58688	302	0.56988	9.06135	0.32595	206	0.09285	4.36825	0.10389	21.33784	0.76756	10.28644	0.24464
Peak31(Sheet1)	179.15111	0.44221	13027.47054	228.61752	244	0.1846	12.12558	0.18448	1004	0.07004	4.67558	0.07798	28.55355	0.43442	11.01016	0.18363
Peak32(Sheet1)	179.15111	0.44221	2042.69001	316.80541	290	70.26566	0.23106	13.99678	139	2.81888	28.20199	3.7799	0.54411	32.95989	66.41061	8.90098
Peak33(Sheet1)	179.15111	0.44221	14217.99325	267.31008	767	0.04098	2.74998	0.04389	51	0.33738	16.58806	0.26398	6.47571	0.10335	39.0619	0.62163
Peak34(Sheet1)	179.15111	0.44221	20534.1791	353.95537	900	0.14075	8.95677	0.14634	471	0.03435	2.17574	0.0352	21.09159	0.34461	5.12349	0.08288
Peak35(Sheet1)	179.15111	0.44221	13340.96426	173.88944	233	0.21717	6.11393	0.1853	184	0.08038	2.81689	0.09726	14.3972	0.43635	6.63328	0.22904
Peak36(Sheet1)	179.15111	0.44221	13524.96781	262.69184	243	0.1498	7.84447	0.14235	180	0.13528	7.33441	0.1089	18.47232	0.3352	17.27121	0.25645
Peak37(Sheet1)	179.15111	0.44221	21522.01776	282.49207	150	0.04776	3.59188	0.04817	276	0.12098	7.28001	0.1217	8.45824	0.11342	17.1431	0.28659
Peak38(Sheet1)	179.15111	0.44221	20681.96388	398.34179	982	0.12655	8.4446	0.13782	122	0.04206	3.01706	0.04679	19.88551	0.32453	7.10464	0.11018
Peak39(Sheet1)	179.15111	0.44221	3122.86282	2994.22441	511	0.93996	6.7669	0.88959	239	1.63681	7.99597	1.60006	15.93484	2.09482	18.82907	3.76785

Peak40(Sheet1)	179.15111	0.44221	8533.59102	2684.24122	511	0.31218	7.26941	0.24909	233	1.87204	10.30416	0.43588	17.11814	0.58655	24.26443	1.02641
Peak41(Sheet1)	179.15111	0.44221	1985.69405	806.22414	869	1.24537	2.96868	0.87514	103	0.44579	0.79212	0.30928	6.99071	2.0608	1.8653	0.72829
Peak42(Sheet1)	179.15111	0.44221	16897.60957	308.85855	859	0.2515	9.7378	0.20359	101	0.07892	3.80553	0.06118	22.93077	0.47941	8.96133	0.14406
Peak43(Sheet1)	179.15111	0.44221	15137.732	381.95199	388	0.13771	6.85132	0.14671	277	0.06627	3.31034	0.07076	16.13362	0.34548	7.79524	0.16662
Peak44(Sheet1)	179.15111	0.44221	15984.64231	240.6303	153	0.07376	4.80275	0.08099	318	0.13218	9.99118	0.13806	11.30962	0.19072	23.52742	0.3251
Peak45(Sheet1)	179.15111	0.44221	18730.74782	343.92571	613	0.12187	7.9642	0.12808	473	0.04815	3.16227	0.05083	18.75425	0.30161	7.44657	0.11968
Peak46(Sheet1)	179.15111	0.44221	20103.65364	357.37461	163	0.12649	7.36043	0.1395	264	0.052	3.74213	0.05491	17.33249	0.3285	8.81204	0.1293
Peak47(Sheet1)	179.15111	0.44221	14312.41571	242.5544	900	0.13489	9.24424	0.14354	639	0.07586	5.20925	0.0792	21.76852	0.33802	12.26684	0.18649
Peak48(Sheet1)	179.15111	0.44221	20649.0502	284.28276	275	0.04167	2.68486	0.04435	133	0.12089	7.91589	0.12702	6.32237	0.10443	18.64049	0.29911
Peak49(Sheet1)	179.15111	0.44221	16194.66975	268.95787	850	0.05454	2.6856	0.06321	461	0.29776	9.46392	0.24261	6.3241	0.14886	22.28583	0.57131
Peak50(Sheet1)	179.15111	0.44221	19630.70582	279.83361	892	0.0595	3.84801	0.05872	564	0.10695	6.14807	0.11506	9.06138	0.13828	14.47759	0.27094
Peak51(Sheet1)	179.15111	0.44221	17676.96292	333.30115	880	0.26883	9.22468	0.22466	105	0.05984	2.93407	0.05504	21.72247	0.52903	6.90921	0.1296
Peak52(Sheet1)	179.15111	0.44221	4977.40918	261.032	848	0.29051	6.45913	0.2812	455	0.61322	7.28701	0.30053	15.21009	0.66218	17.1596	0.7077
Peak53(Sheet1)	179.15111	0.44221	11649.69564	239.72193	910	0.05869	1.69593	0.0588	442	0.27247	8.83729	0.31987	3.99361	0.13846	20.81022	0.75325
Peak54(Sheet1)	179.15111	0.44221	5191.29985	108.81791	901	0.66998	10.47581	0.27043	431	0.12187	1.96452	0.13852	24.66865	0.63681	4.6261	0.3262
Peak55(Sheet1)	179.15111	0.44221	22668.67382	187.58282	142	0.05996	2.53421	0.05431	318	0.07599	3.63479	0.07362	5.96762	0.1279	8.55929	0.17335
Peak56(Sheet1)	179.15111	0.44221	15748.69408	257.00221	30	0.07437	5.77867	0.08077	92	0.11116	8.69501	0.1197	13.60773	0.1902	20.47517	0.28186
Peak57(Sheet1)	179.15111	0.44221	16557.60602	383.29511	551	0.12346	6.48659	0.13035	351	0.06049	3.17709	0.06398	15.27476	0.30696	7.48149	0.15066
Peak58(Sheet1)	179.15111	0.44221	11936.58624	226.86818	258	0.07488	4.75791	0.08114	299	0.20688	12.75465	0.2326	11.20402	0.19107	30.0349	0.54774
Peak59(Sheet1)	179.15111	0.44221	9515.91997	203.05046	726	0.31456	4.50183	0.21349	51	0.10216	1.9766	0.10414	10.601	0.50274	4.65453	0.24523
Peak60(Sheet1)	179.15111	0.44221	14307.91324	228.08395	159	0.0971	6.74733	0.1077	177	0.12014	8.78984	0.12064	15.88875	0.25362	20.69848	0.28408
Peak61(Sheet1)	179.15111	0.44221	14259.10204	297.15187	40	0.13195	5.32297	0.12716	18	0.07669	3.1105	0.07392	12.53463	0.29943	7.32467	0.17408
Peak62(Sheet1)	179.15111	0.44221	-1234.05319	207.3265	303	0.81482	4.96921	0.65004	119	0.63036	4.91718	0.56846	11.70159	1.53074	11.57907	1.33863
Peak63(Sheet1)	179.15111	0.44221	13215.01828	299.669	419	0.15617	8.38197	0.16174	124	0.07627	4.19826	0.08122	19.73804	0.38087	9.88614	0.19125
Peak64(Sheet1)	179.15111	0.44221	7809.96947	216.29571	880	0.40665	7.16852	0.31071	549	0.23692	4.91661	0.19922	16.88058	0.73166	11.57773	0.46913
Peak65(Sheet1)	179.15111	0.44221	9445.1239	1501.70448	757	1.04466	6.95624	0.37155	125	0.30705	4.82548	0.14087	16.38069	0.87494	11.36314	0.33172
Peak66(Sheet1)	179.15111	0.44221	10481.11498	140.40004	277	0.21256	8.98681	0.21175	185	0.09998	4.71223	0.09206	21.16231	0.49864	11.09645	0.21679
Peak67(Sheet1)	179.15111	0.44221	8677.30037	232.80326	194	0.18356	5.13301	0.1853	33	0.2165	8.24144	0.2177	12.08733	0.43634	19.40711	0.51265
Peak68(Sheet1)	179.15111	0.44221	9717.18237	334.66624	214	0.10013	2.97517	0.10857	31	0.25496	7.60299	0.24231	7.006	0.25566	17.90368	0.57061
Peak69(Sheet1)	179.15111	0.44221	5441.1546	66.55161	388	0.29298	4.72911	0.26473	236	0.71096	9.32265	0.61481	11.1362	0.62339	21.95316	1.44776
Peak70(Sheet1)	179.15111	0.44221	11606.59205	116.83217	301	0.1242	2.64706	0.11644	318	0.13836	2.89248	0.12547	6.23336	0.2742	6.81128	0.29546
Peak71(Sheet1)	179.15111	0.44221	9396.5955	194.52873	169	0.09891	2.84948	0.10303	236	0.30303	8.49942	0.32735	6.71001	0.24263	20.01461	0.77084
Peak72(Sheet1)	179.15111	0.44221	9000.63211	191.99253	246	0.25073	9.08804	0.23664	331	0.10873	4.05869	0.1027	21.40069	0.55725	9.55748	0.24183
Peak73(Sheet1)	179.15111	0.44221	6870.27359	309.88088	183	0.28206	6.58119	0.30326	188	0.18706	4.60103	0.19395	15.49752	0.71412	10.83459	0.45671
Peak74(Sheet1)	179.15111	0.44221	8838.93711	380.43971	935	0.15369	3.56496	0.15345	400	0.17869	3.99381	0.17212	8.39484	0.36134	9.40469	0.40532
Peak75(Sheet1)	179.15111	0.44221	6552.03437	421.7744	916	0.16172	2.14196	0.19897	111	0.36564	3.97676	0.33851	5.04394	0.46853	9.36455	0.79713
Peak76(Sheet1)	179.15111	0.44221	7054.35965	194.23882	923	0.2683	10.03653	0.24029	116	0.25034	10.99497	0.25753	23.63421	0.56585	25.89117	0.60643
Peak77(Sheet1)	179.15111	0.44221	7773.53924	147.79711	798	0.40467	7.88309	0.37634	158	0.22023	3.13215	0.18712	18.56325	0.88622	7.37564	0.44062
Peak78(Sheet1)	179.15111	0.44221	7710.63504	164.64719	437	0.0886	1.49969	0.07985	277	0.30847	6.56564	0.29081	3.53149	0.18802	15.46091	0.68481
Peak79(Sheet1)	179.15111	0.44221	10234.99372	114.34859	865	0.11237	2.02561	0.09967	685	0.17483	3.12537	0.15675	4.76994	0.23471	7.35968	0.36913
Peak80(Sheet1)	179.15111	0.44221	7581.14968	246.69326	798	0.40148	9.25507	0.30868	150	0.26525	3.9353	0.1916	21.79403	0.72688	9.26691	0.45119
Peak81(Sheet1)	179.15111	0.44221	8886.05023	--	218	199.58254	0.22461	40.01101	277	--	3.60608E-7	--	0.52892	94.21874	8.49167E-7	--
Peak82(Sheet1)	179.15111	0.44221	12319.72166	775.18698	163	0.10777	1.22057	0.10101	206	0.12603	1.46525	0.12137	2.87421	0.23785	3.4504	0.28581
Peak83(Sheet1)	179.15111	0.44221	5706.13098	307.60211	798	0.76286	17.35395	0.63381	467	0.0893	2.18342	0.09486	40.86543	1.4925	5.14156	0.22338
Peak84(Sheet1)	179.15111	0.44221	12559.46516	314.31179	900	0.37801	10.08244	0.30002	57	0.03932	1.19686	0.03708	23.74234	0.7065	2.81838	0.08732
Peak85(Sheet1)	179.15111	0.44221	-226.53252	44.85043	879	22.38639	114.78035	22.15222	574	1.35893	14.13625	1.23657	270.28708	52.1645	33.28833	2.91189
Peak86(Sheet1)	179.15111	0.44221	11132.08521	218.2209	694	0.1217	8.57034	0.13498	767	0.13633	9.51583	0.15073	20.18161	0.31785	22.40806	0.35495

Peak87(Sheet1)	179.15111	0.44221	9321.03883	366.45312	233	0.13101	1.40563	0.11437	242	0.18269	2.03704	0.16048	3.31	0.26931	4.79687	0.37791
Peak88(Sheet1)	179.15111	0.44221	10148.25572	186.34695	853	0.12314	1.16345	0.10166	52	0.17032	1.65935	0.14082	2.73971	0.23939	3.90747	0.33161
Peak89(Sheet1)	179.15111	0.44221	10164.99019	1484.14688	224	5.86212	0.29097	1.221	283	46.11495	0.24199	6.28586	0.68519	2.87522	0.56984	14.80206
Peak90(Sheet1)	179.15111	0.44221	5998.28076	298.92439	174	0.08379	2.74661	0.09374	195	0.80177	28.14072	1.01663	6.46777	0.22075	66.26632	2.39399
Peak91(Sheet1)	179.15111	0.44221	11725.07907	1553.54306	258	0.92894	0.35526	0.27158	317	0.40147	0.42381	0.13608	0.83657	0.63952	0.998	0.32045
Peak92(Sheet1)	179.15111	0.44221	2596.26479	164.15115	916	0.25872	10.39118	0.5084	13	0.61086	16.96025	1.15035	24.46936	1.1972	39.93834	2.70886
Peak93(Sheet1)	179.15111	0.44221	-424.6206	139.51617	212	23134.36659	0.1923	2428.60926	274	10.76794	7.06119	6.26274	0.45284	5718.93776	16.62784	14.74763
Peak94(Sheet1)	179.15111	0.44221	6953.79088	233.63067	766	0.26201	7.19239	0.23338	417	0.48267	8.13984	0.37208	16.93679	0.54957	19.16785	0.87618
Peak95(Sheet1)	179.15111	0.44221	3928.29864	76.44999	212	0.558	37.47992	0.46964	280	0.32574	18.33531	0.32581	88.25846	1.10592	43.17636	0.76722
Peak96(Sheet1)	179.15111	0.44221	755.99842	166.89966	394	4.02201	6.241	3.10577	228	2.83152	6.13549	1.79642	14.69644	7.31352	14.44797	4.23025
Peak97(Sheet1)	179.15111	0.44221	5904.44746	183.30613	742	0.37552	9.59076	0.36098	583	0.27675	9.27603	0.26154	22.58451	0.85004	21.84337	0.61588
Peak98(Sheet1)	179.15111	0.44221	-1035.54146	206.75573	171	0.72233	12.72527	1.50023	228	2.82407	26.94035	3.50068	29.96573	3.53277	63.43969	8.24347
Peak99(Sheet1)	179.15111	0.44221	2771.07662	284.14487	382	0.81085	13.62405	0.74958	227	0.39598	7.02218	0.38362	32.08218	1.76512	16.53597	0.90335
Peak100(Sheet1)	179.15111	0.44221	5834.5481	245.03653	118	0.47591	8.48572	0.37713	148	0.20556	4.95871	0.19785	19.98235	0.88806	11.67686	0.46591
Peak101(Sheet1)	179.15111	0.44221	7242.86728	363.58732	900	0.26468	9.266	0.37356	46	0.11241	2.89366	0.12015	21.81976	0.87967	6.81406	0.28294
Peak102(Sheet1)	179.15111	0.44221	2655.60845	140.02565	922	0.54738	43.03555	1.30746	16	0.26914	8.90151	0.23018	101.34098	3.07884	20.96146	0.54202
Peak103(Sheet1)	179.15111	0.44221	5300.89485	265.10641	694	0.3427	7.83873	0.39983	327	0.19404	3.86537	0.19232	18.45881	0.94152	9.10224	0.45289
Peak104(Sheet1)	179.15111	0.44221	4690.51044	179.94923	730	0.2059	2.68454	0.24352	583	0.46013	7.15964	0.32848	6.3216	0.57346	16.85966	0.77351
Peak105(Sheet1)	179.15111	0.44221	8940.29842	232.97026	358	0.13517	4.27245	0.13088	350	0.19284	5.99984	0.19683	10.06084	0.3082	14.12855	0.46351
Peak106(Sheet1)	179.15111	0.44221	7440.64574	--	737	0.56036	4.19108	0.1951	494	0.08719	0.83934	0.06868	9.86925	0.45942	1.97649	0.16172
Peak107(Sheet1)	179.15111	0.44221	7650.85102	358.84106	736	0.31023	3.57907	0.31474	591	0.10695	1.15765	0.1057	8.42807	0.74116	2.72606	0.2489
Peak108(Sheet1)	179.15111	0.44221	4459.37943	1350.25032	746	2.55664	7.0948	0.94501	123	0.48598	4.24399	0.31819	16.70698	2.22533	9.99383	0.74927
Peak109(Sheet1)	179.15111	0.44221	5501.82144	155.81824	127	0.34394	2.67307	0.32888	150	0.28551	2.35203	0.27585	6.29459	0.77444	5.5386	0.64957
Peak110(Sheet1)	179.15111	0.44221	8583.82788	179.58848	213	0.11244	1.9684	0.09926	230	0.25571	4.40891	0.22637	4.63522	0.23373	10.38219	0.53306
Peak111(Sheet1)	179.15111	0.44221	3825.95123	306.65621	944	0.66213	10.57315	0.67464	145	0.23327	3.57955	0.24538	24.89788	1.58867	8.4292	0.57783
Peak112(Sheet1)	179.15111	0.44221	8666.3134	221.72877	726	0.08855	3.47905	0.08446	40	0.31344	15.6471	0.38493	8.19254	0.1989	36.8461	0.90644
Peak113(Sheet1)	179.15111	0.44221	7684.86636	225.68005	683	0.1029	2.10464	0.09937	337	0.3804	7.07572	0.36889	4.95604	0.23401	16.66204	0.86866
Peak114(Sheet1)	179.15111	0.44221	10718.33494	240.32972	899	0.29462	9.10635	0.32317	658	0.06755	2.26263	0.06678	21.44381	0.76101	5.32808	0.15725
Peak115(Sheet1)	179.15111	0.44221	8256.09965	268.91604	273	0.10258	3.42657	0.1077	318	0.28774	10.24762	0.32895	8.06895	0.25362	24.13129	0.77462
Peak116(Sheet1)	179.15111	0.44221	11455.78924	365.57161	49	0.06829	2.3317	0.06989	359	0.26839	7.80702	0.23409	5.49072	0.16459	18.38412	0.55125
Peak117(Sheet1)	179.15111	0.44221	5049.54864	186.25457	408	0.33145	9.01427	0.33717	338	0.30593	6.64341	0.24393	21.22697	0.79397	15.64404	0.57441
Peak118(Sheet1)	179.15111	0.44221	7836.33625	217.91436	141	0.12722	4.18131	0.12605	72	0.29981	8.96862	0.31086	9.84623	0.29683	21.1195	0.73201
Peak119(Sheet1)	179.15111	0.44221	7663.212	44.36215	526	1969.57013	15168.12231	44158.52847	236	0.00718	0.64756	0.00499	35718.19846	103985.388	1.52488	0.01176
Peak120(Sheet1)	179.15111	0.44221	3498.3692	229.12339	592	0.25259	8.54019	0.53034	277	0.36846	8.1256	0.49678	20.11061	1.24886	19.13432	1.16983
Peak121(Sheet1)	179.15111	0.44221	10460.23833	416.82993	491	0.32145	7.86384	0.259	101	0.07841	2.58563	0.08519	18.51793	0.60989	6.0887	0.20062
Peak122(Sheet1)	179.15111	0.44221	9054.7375	398.05109	306	0.38491	8.25517	0.33888	692	0.08253	2.2437	0.08701	19.43944	0.798	5.28351	0.2049
Peak123(Sheet1)	179.15111	0.44221	6637.28506	281.09423	199	0.33505	8.85328	0.3449	248	0.1621	4.42634	0.1767	20.84787	0.81217	10.42324	0.41609
Peak124(Sheet1)	179.15111	0.44221	6244.32367	193.28935	396	0.5505	22.48698	0.54659	338	0.07751	2.16055	0.08481	52.9528	1.28713	5.0877	0.19972
Peak125(Sheet1)	179.15111	0.44221	6845.39358	327.89286	540	0.21196	4.82424	0.20631	328	0.21459	5.37739	0.22938	11.36021	0.48582	12.66279	0.54014
Peak126(Sheet1)	179.15111	0.44221	8070.59324	324.89684	440	0.11228	3.69409	0.12323	93	0.3391	9.30402	0.32711	8.69891	0.29018	21.90929	0.77027
Peak127(Sheet1)	179.15111	0.44221	7970.31397	192.41373	897	0.29516	10.3103	0.30921	674	0.12325	4.67755	0.12376	24.2789	0.72813	11.01478	0.29144
Peak128(Sheet1)	179.15111	0.44221	7727.03289	388.57748	745	0.18369	4.69006	0.19806	348	0.19016	4.91572	0.20836	11.04424	0.46639	11.57563	0.49064
Peak129(Sheet1)	179.15111	0.44221	5601.35206	237.95676	183	1.00304	15.5971	0.64413	604	0.06083	0.87137	0.05193	36.72835	1.51682	2.05192	0.12228
Peak130(Sheet1)	179.15111	0.44221	4052.95147	296.56747	907	0.20011	1.6015	0.20944	113	0.5596	5.14427	0.54477	3.77125	0.49318	12.11384	1.28285
Peak131(Sheet1)	179.15111	0.44221	7115.70249	243.35158	311	0.24126	8.53722	0.25353	325	0.19468	6.6971	0.19856	20.10361	0.59701	15.77046	0.46757
Peak132(Sheet1)	179.15111	0.44221	7573.64484	219.81209	263	0.19292	8.11869	0.20389	892	0.19454	7.98268	0.2003	19.11806	0.48011	18.79777	0.47166
Peak133(Sheet1)	179.15111	0.44221	8600.87198	209.87415	18	0.35052	7.39324	0.27112	199	0.08195	1.78255	0.0727	17.40975	0.63843	4.19758	0.1712
Peak134(Sheet1)	179.15111	0.44221	8373.36581	319.11487	481	0.17058	4.15597	0.16626	121	0.17817	4.35375	0.17445	9.78656	0.39151	10.2523	0.41081

Peak135(Sheet1)	179.15111	0.44221	8416.84827	294.00357	771	0.10319	2.39421	0.09975	297	0.38897	6.69979	0.32097	5.63794	0.2349	15.77679	0.75583
Peak136(Sheet1)	179.15111	0.44221	5126.5046	186.21321	872	0.32196	6.22379	0.29282	536	0.56118	6.46978	0.48048	14.65591	0.68954	15.23517	1.13143
Peak137(Sheet1)	179.15111	0.44221	7176.95351	399.70915	599	0.11841	2.81794	0.1275	400	0.31243	8.29207	0.36338	6.63575	0.30023	19.52634	0.8557
Peak138(Sheet1)	179.15111	0.44221	9305.90141	790.74018	839	0.18553	2.02971	0.17854	93	0.13253	1.47986	0.13067	4.77961	0.42043	3.4848	0.3077
Peak139(Sheet1)	179.15111	0.44221	7649.35489	341.1407	449	0.26523	7.57143	0.30115	183	0.13445	3.88349	0.14679	17.82935	0.70916	9.14492	0.34566
Peak140(Sheet1)	179.15111	0.44221	4264.9002	216.37661	194	0.35686	6.81022	0.30847	203	0.27027	9.55195	0.39612	16.03683	0.72639	22.49312	0.93279
Peak141(Sheet1)	179.15111	0.44221	6500.67521	392.34782	395	0.1667	3.81507	0.18171	93	0.40168	7.21274	0.35322	8.98381	0.42789	16.9847	0.83176
Peak142(Sheet1)	179.15111	0.44221	7697.80808	312.77473	627	0.36652	8.05486	0.28864	412	0.13308	3.91503	0.13646	18.96775	0.67969	9.2192	0.32134
Peak143(Sheet1)	179.15111	0.44221	3592.41456	487.05924	896	0.10474	0.66939	0.07517	14	1.50555	13.20934	2.04956	1.57629	0.17701	31.10562	4.82635
Peak144(Sheet1)	179.15111	0.44221	8971.04964	214.28947	11	0.1489	3.16731	0.13589	101	0.17281	3.58509	0.1528	7.45845	0.32	8.44223	0.35981
Peak145(Sheet1)	179.15111	0.44221	8655.32085	250.84256	561	0.17608	3.57489	0.15808	369	0.17176	3.60576	0.1597	8.41823	0.37226	8.49092	0.37607
Peak146(Sheet1)	179.15111	0.44221	6331.44047	366.86941	95	0.27905	6.58908	0.32954	287	0.17766	3.94204	0.19008	15.51609	0.77601	9.28279	0.44762
Peak147(Sheet1)	179.15111	0.44221	6627.45657	358.13009	88	0.23162	4.14525	0.22169	21	0.2409	4.18851	0.2243	9.76132	0.52203	9.86319	0.5282
Peak148(Sheet1)	179.15111	0.44221	5261.49131	181.93411	941	0.29083	8.49125	0.3117	46	0.26294	7.00798	0.25674	19.99536	0.734	16.50252	0.60458
Peak149(Sheet1)	179.15111	0.44221	5706.87099	173.7863	771	0.21751	4.46453	0.21033	585	0.31108	7.73968	0.33636	10.51315	0.4953	18.22556	0.79206
Peak150(Sheet1)	179.15111	0.44221	4489.81035	241.91623	685	0.23483	3.69964	0.21098	808	0.60898	7.83494	0.41609	8.71199	0.49682	18.44988	0.97981
Peak151(Sheet1)	179.15111	0.44221	7012.83757	344.64806	162	0.49044	4.67865	0.42254	854	0.11428	1.45209	0.10949	11.01739	0.99501	3.41942	0.25783
Peak152(Sheet1)	179.15111	0.44221	5978.06029	484.36504	129	0.30012	3.782	0.29435	368	0.31566	3.85639	0.30304	8.90593	0.69314	9.08109	0.7136
Peak153(Sheet1)	179.15111	0.44221	4833.97138	407.95171	480	0.39303	4.64046	0.38604	148	0.35907	4.5306	0.37177	10.92745	0.90906	10.66874	0.87546
Peak154(Sheet1)	179.15111	0.44221	4270.59262	308.03966	121	0.63063	8.27609	0.39647	89	0.18916	2.55638	0.17814	19.4887	0.93361	6.01981	0.41948
Peak155(Sheet1)	179.15111	0.44221	4876.14216	417.19967	722	0.38116	3.91035	0.30697	677	0.40362	4.40395	0.35496	9.20817	0.72285	10.37051	0.83586
Peak156(Sheet1)	179.15111	0.44221	5576.2623	237.27586	701	0.29189	4.01706	0.23725	307	0.31236	4.64211	0.28784	9.45944	0.55867	10.93133	0.6778
Peak157(Sheet1)	179.15111	0.44221	6607.46804	406.36879	394	0.08235	1.25538	0.07782	31	0.53183	8.81055	0.35899	2.9562	0.18325	20.74726	0.84536
Peak158(Sheet1)	179.15111	0.44221	6312.75238	531.80477	352	0.14652	2.16166	0.15462	564	0.4295	5.25217	0.3559	5.09033	0.36409	12.36792	0.83808
Peak159(Sheet1)	179.15111	0.44221	6301.05043	623.08731	122	0.39755	1.41033	0.30999	686	0.18476	0.82904	0.15885	3.32107	0.72996	1.95223	0.37407
Peak160(Sheet1)	179.15111	0.44221	3248.82185	344.613	456	0.19718	1.59178	0.17827	379	0.69864	8.14177	0.48704	3.74836	0.41979	19.1724	1.14689
Peak161(Sheet1)	179.15111	0.44221	7431.0451	2029.02427	189	0.19767	0.76174	0.18536	307	0.21105	0.71429	0.16425	1.79375	0.43648	1.68202	0.38677
Peak162(Sheet1)	179.15111	0.44221	5640.09223	295.62335	74	0.17157	2.7105	0.16182	831	0.44343	5.97329	0.34599	6.38274	0.38106	14.06603	0.81474
Peak163(Sheet1)	179.15111	0.44221	3767.0461	175.04186	962	0.4625	12.06702	0.44621	134	0.36524	7.39267	0.40602	28.41566	1.05073	17.4084	0.95611
Peak164(Sheet1)	179.15111	0.44221	1804.61253	254.32681	125	1.19164	8.70339	0.68019	692	0.22784	7.01955	0.58345	20.49493	1.60172	16.52977	1.37391
Peak165(Sheet1)	179.15111	0.44221	4535.12981	570.87472	511	0.74657	5.26561	0.46779	57	0.17719	1.48448	0.16672	12.39956	1.10155	3.49569	0.39259
Peak166(Sheet1)	179.15111	0.44221	2799.11715	348.25872	941	0.16893	11.24055	0.94718	78	0.31618	2.59552	0.26266	26.46947	2.23044	6.11198	0.61851
Peak167(Sheet1)	179.15111	0.44221	7965.68641	1.06308E10	450	2.79497E10	0.00429	--	372	228.14282	2.89536E-8	273162.11845	0.01011	--	6.81804E-8	643247.63207
Peak168(Sheet1)	179.15111	0.44221	2177.80964	195.24946	203	0.49065	11.66779	0.57799	912	0.72374	9.37128	0.51785	27.47555	1.36105	22.06768	1.21945
Peak169(Sheet1)	179.15111	0.44221	5504.37588	331.62217	19	0.42785	8.77806	0.4202	575	0.1681	3.53775	0.17595	20.67076	0.98949	8.33076	0.41434
Peak170(Sheet1)	179.15111	0.44221	4392.34422	221.90505	838	0.38057	7.86737	0.34473	544	0.39445	7.87587	0.35007	18.52623	0.81177	18.54626	0.82436
Peak171(Sheet1)	179.15111	0.44221	8037.14144	2013.56654	695	0.61469	0.40545	0.22156	242	0.41782	0.47822	0.16146	0.95477	0.52173	1.12611	0.38022
Peak172(Sheet1)	179.15111	0.44221	3901.4378	603.45398	948	0.5736	1.35082	0.63505	64	5.40968	0.30712	0.88803	3.18093	1.49544	0.72321	2.09116
Peak173(Sheet1)	179.15111	0.44221	3594.80475	287.1127	765	0.35602	2.87777	0.3827	573	0.52488	3.36978	0.46303	6.77662	0.90118	7.93523	1.09035
Peak174(Sheet1)	179.15111	0.44221	3917.1862	1679.46846	875	0.48208	0.80464	0.33814	638	0.35675	0.69243	0.27779	1.89479	0.79625	1.63054	0.65414
Peak175(Sheet1)	179.15111	0.44221	2343.04818	391.69589	110	0.81106	5.00604	0.632	41	0.81374	4.87583	0.60985	11.78832	1.48824	11.48171	1.43608
Peak176(Sheet1)	179.15111	0.44221	1230.35746	260.11985	724	0.65986	1.84638	0.31924	125	0.55892	3.12248	0.39305	4.3479	0.75175	7.35287	0.92556
Peak177(Sheet1)	179.15111	0.44221	4688.66783	1167.00378	988	0.38866	1.39776	0.31605	635	0.42585	1.52652	0.3504	3.29148	0.74425	3.59467	0.82513
Peak178(Sheet1)	179.15111	0.44221	2456.72849	170.57939	512	0.37739	9.79896	0.30408	376	0.33316	4.42811	0.3471	23.07479	0.71604	10.42741	0.81736
Peak179(Sheet1)	179.15111	0.44221	5345.24657	435.23295	956	0.12921	1.77774	0.12757	400	0.74814	7.94974	0.41132	4.18627	0.3004	18.7202	0.96859
Peak180(Sheet1)	179.15111	0.44221	3167.15657	246.45282	477	0.45633	2.09191	0.35662	184	0.42999	2.31889	0.4045	4.92607	0.83978	5.46058	0.95252
Peak181(Sheet1)	179.15111	0.44221	4689.11192	380.47562	329	0.19066	3.10697	0.19987	72	0.62372	8.08559	0.42197	7.31635	0.47067	19.0401	0.99366
Peak182(Sheet1)	179.15111	0.44221	3351.99379	198.71114	143	0.39938	7.60869	0.35438	117	0.33859	4.39034	0.31166	17.91711	0.8345	10.33845	0.73391

Peak183(Sheet1)	179.15111	0.44221	2043.00178	83.60911	872	0.30549	5.85395	0.28348	661	0.28378	38.45712	0.98212	13.78499	0.66755	90.55959	2.31272
Peak184(Sheet1)	179.15111	0.44221	2536.58521	1.83921E8	471	0.01278	8.87346E-11	0.62449	255	265.82984	0.23622	65.68351	2.08954E-10	1.47057	0.55626	154.67285
Peak185(Sheet1)	179.15111	0.44221	1802.0206	115.46255	511	0.69961	8.94505	0.30071	384	0.36402	3.52642	0.40756	21.06398	0.70812	8.30407	0.95973
Peak186(Sheet1)	179.15111	0.44221	4276.59349	53.17595	471	0.25157	40.37579	0.42992	258	0.33497	20.77721	0.28624	95.07773	1.01238	48.92658	0.67404
Peak187(Sheet1)	179.15111	0.44221	5423.8621	239.8821	93	0.14641	2.30306	0.13928	72	0.56462	7.38722	0.49614	5.4233	0.32798	17.39558	1.16831
Peak188(Sheet1)	179.15111	0.44221	5017.18351	389.60776	887	0.17369	2.6879	0.17669	341	0.59181	7.52212	0.42269	6.32951	0.41607	17.71324	0.99536
Peak189(Sheet1)	179.15111	0.44221	4198.08652	358.20105	668	0.23276	3.73164	0.24255	499	0.62367	8.56877	0.43132	8.78733	0.57115	20.17792	1.01569
Peak190(Sheet1)	179.15111	0.44221	2839.27169	130.5393	797	0.3009	10.12203	0.44059	420	0.43059	16.27221	0.47007	23.83557	1.03752	38.31813	1.10694
Peak191(Sheet1)	179.15111	0.44221	2443.42741	412.06366	193	0.77808	4.5406	0.56967	412	0.77482	4.13371	0.52752	10.69229	1.34147	9.73414	1.24222
Peak192(Sheet1)	179.15111	0.44221	5056.57825	318.17257	872	0.15895	2.38271	0.15246	339	0.38392	7.41922	0.3727	5.61086	0.35901	17.47092	0.87764
Peak193(Sheet1)	179.15111	0.44221	4156.96579	383.17033	632	0.30269	7.917	0.4813	508	0.23444	3.30432	0.23884	18.64311	1.13337	7.78108	0.56244
Peak194(Sheet1)	179.15111	0.44221	2100.23244	247.76842	855	0.76985	6.77258	0.51092	297	0.67023	8.84057	0.6496	15.9482	1.20311	20.81796	1.52969
Peak195(Sheet1)	179.15111	0.44221	3139.43995	311.01873	706	0.61788	4.80323	0.51285	23	0.4861	4.569	0.4804	11.31074	1.20766	10.75917	1.13126
Peak196(Sheet1)	179.15111	0.44221	3527.15312	202.97621	163	0.28273	8.84976	0.38646	133	0.38416	6.0078	0.34291	20.8396	0.91003	14.14728	0.80749
Peak197(Sheet1)	179.15111	0.44221	3347.03695	498.50888	564	0.57079	3.87611	0.42072	735	0.54725	3.79834	0.41619	9.12753	0.99071	8.94442	0.98005
Peak198(Sheet1)	179.15111	0.44221	1645.50977	246.46597	655	1.39441	9.24279	0.81733	94	0.83957	6.88796	0.6333	21.76511	1.92465	16.21992	1.49131
Peak199(Sheet1)	179.15111	0.44221	4746.56768	302.36071	320	0.18074	2.28987	0.16122	379	0.62102	7.20735	0.44689	5.39222	0.37964	16.97201	1.05235
Peak200(Sheet1)	179.15111	0.44221	3460.43019	439.81296	264	0.715	8.0696	0.59471	935	0.32051	2.64961	0.25752	19.00245	1.40044	6.23934	0.60642

5. Gaussian surface fitting code (Generated by ChatGPT)

```
****************************************************

import numpy as np

from scipy.optimize import curve_fit


# Define the Gaussian function

def gaussian_surface(xy, A, x0, y0, sigma_x, sigma_y):

    x, y = xy

    return A * np.exp(-(((x - x0) ** 2) / (2 * sigma_x ** 2)) - (((y - y0) ** 2) / (2 * sigma_y ** 2)))


# Generate example data (replace with your actual data)

x_data = ...

y_data = ...

z_data = ...


# Perform the curve fitting

initial_guess = [1.0, 0.0, 0.0, 1.0, 1.0]  # Initial parameter guess

popt, pcov = curve_fit(gaussian_surface, (x_data, y_data), z_data, p0=initial_guess)


# Extract the fitted parameters
```

```
A_fit, x0_fit, y0_fit, sigma_x_fit, sigma_y_fit = popt

# Evaluate the fitted Gaussian surface
x_eval = ...  # Replace with the x-values at which you want to evaluate the surface
y_eval = ...  # Replace with the y-values at which you want to evaluate the surface
z_fit = gaussian_surface((x_eval, y_eval), A_fit, x0_fit, y0_fit, sigma_x_fit, sigma_y_fit)

# Print the fitted parameters
print("Fitted Amplitude (A):", A_fit)
print("Fitted x0:", x0_fit)
print("Fitted y0:", y0_fit)
print("Fitted Sigma_x:", sigma_x_fit)
print("Fitted Sigma_y:", sigma_y_fit)
```

****

Make sure to replace x_data, y_data, and z_data with your actual data arrays. Also, provide appropriate values or arrays for x_eval and y_eval to evaluate the fitted surface at desired points.

This code assumes that you have NumPy and SciPy libraries installed. If you don't have them, you can install them using pip install numpy scipy.

Please note that this is a basic example, and you may need to adjust it according to your specific requirements and data structure.

6. Real sample #3: mixture

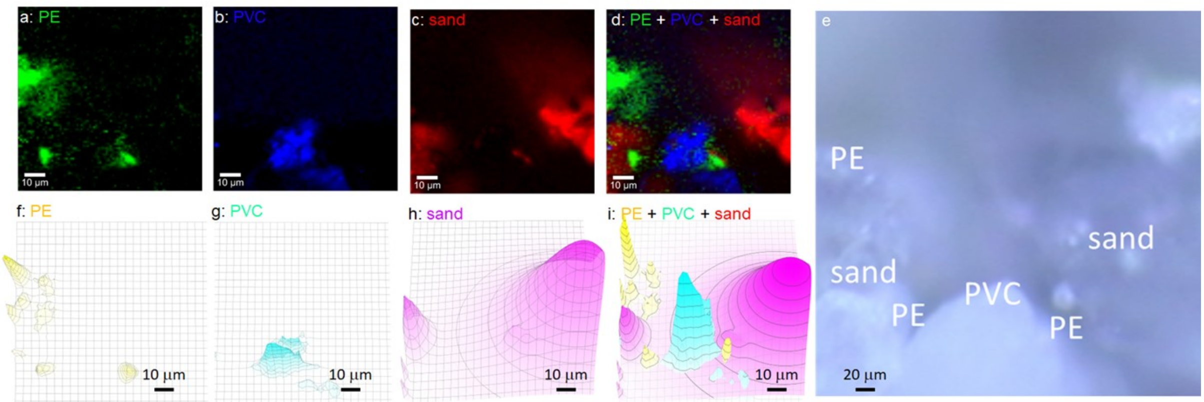

Figure S4. Raman images (a-d), re-constructed images (f-i) and photo image (e). The sample was a mixture of sand, PE and PVC. Raman images (a-d) are mapped via their characteristic peaks at ~1059

cm^{-1} for PE, ~695 cm^{-1} for PVC, and ~520 cm^{-1} for sand, and re-construct as (f-i), respectively. (d, i) merges them to show the mixture of plastics and sand. (e) shows a photo image for comparison with the items identified by Raman.

A mixture is analysed in this section, including PE, PVC and sand [1]. The mapping and imaging are based on their characteristic peaks towards identification. The images (a-c) can be re-constructed as (f-h), individually. The mixture can be visualised in (d) and (i), before and after the re-construction. The imaging and assignment certainty can be significantly increased by the image re-construction. Compared to the photo image in (e), the advantage of Raman imaging is obviously demonstrated, along with the image re-construction. That is, the reported approach can effectively identify and visualise the mixture containing the different plastics and other items, which cannot be achieved in the photo image.

Reference

1. Z. Sobhani, M. Al Amin, R. Naidu, M. Megharaj and C. Fang, *Analytica Chimica Acta*, 2019, **1077**, 191-199.