Supplementary Information

# Statistical fusion identification of dairy products based on extracted Raman spectroscopy

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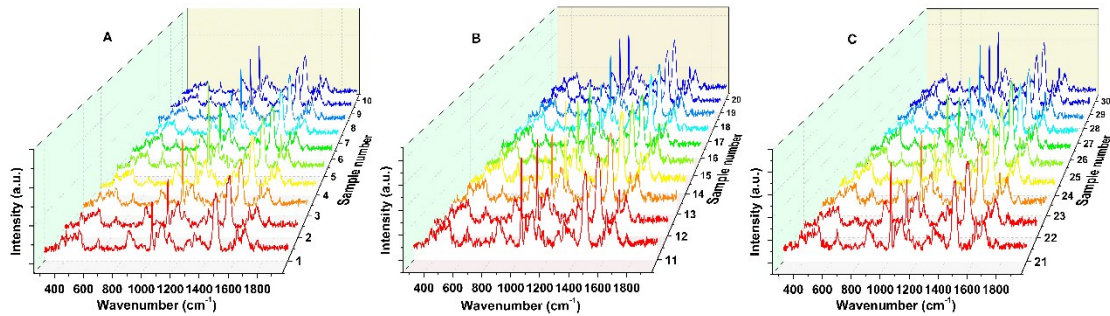*Correspondence to Prof. Zheng-Yong Zhang. E-mail: zyzhang@nufe.edu.cn
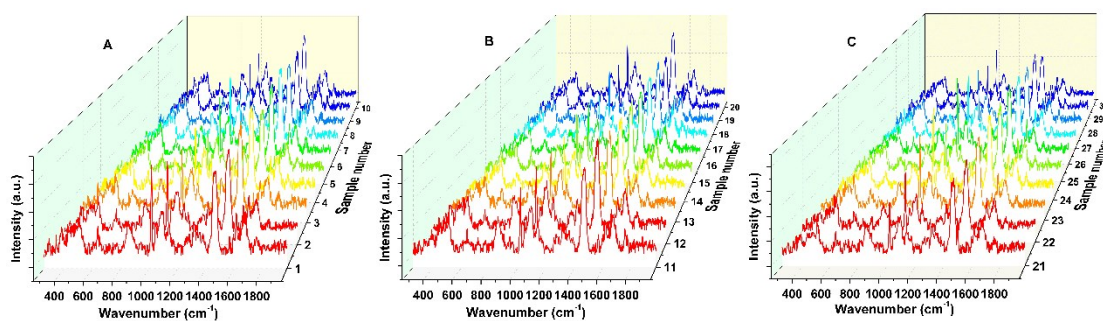
Figure S1 Raman spectra of momchilovtsi pasteurized heat-treated flavor yoghurt products from Bright Dairy & Food Co., Ltd. (A) sample number 1-10, (B) sample number 11-20, and (C) sample number 21-30.
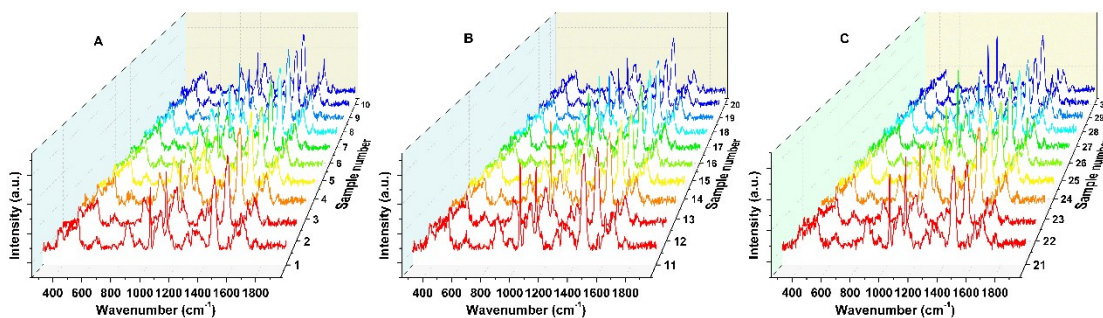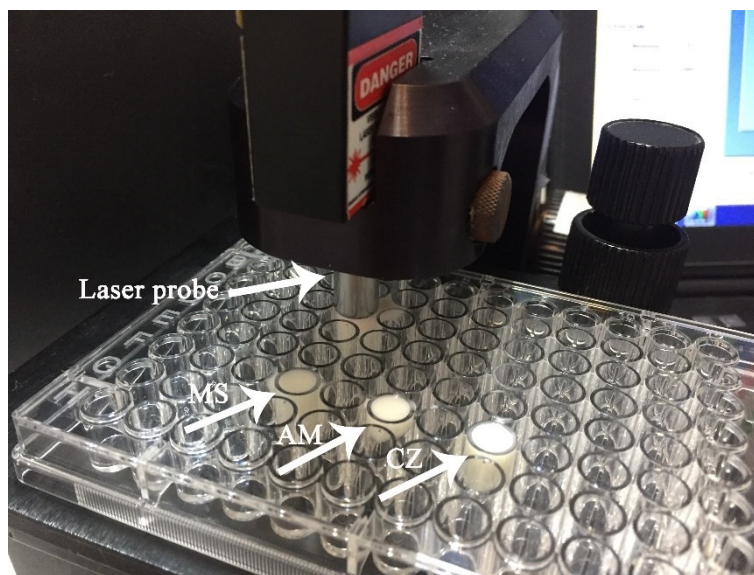

Figure S2 Raman spectra of ambpoeial pasteurized heat-treated flavor yoghurt products from Inner Mongolia Yili Industrial Group Co., Ltd. (A) sample number 1-

10, (B) sample number 11-20, and (C) sample number 21-30.

Figure S3 Raman spectra of ChunZhen pasteurized heat-treated flavor yoghurt products from Mengniu Dairy Group Co. Ltd. (A) sample number 1-10, (B) sample number 11-20, and (C) sample number 21-30.

Figure S4 Schematic diagram of test and sample.

(MS represents the momchilovtsi pasteurized heat-treated flavor yoghurt products from Bright Dairy & Food Co., Ltd. AM represents the ambpoeial pasteurized heat-treated flavor yoghurt products from Inner Mongolia Yili Industrial Group Co., Ltd. CZ represents the ChunZhen pasteurized heat-treated flavor yoghurt products from Mengniu Dairy Group Co. Ltd.)

The statistical control chart can be realized using the following individual and moving range chart formulae. For the individual (x) control chart, the formula is as follows[1]:

$$UCL_x = \overline{x} + 2.66\overline{MR}$$
$$CL_x = \overline{x}$$
$$LCL_x = \overline{x} - 2.66\overline{MR}$$

For the moving range (MR) control chart, the formula is as follows:

$$UCL_{MR} = 3.267\overline{MR}$$
$$CL_{MR} = \overline{MR}$$
$$LCL_{MR} = 0$$

In the formulae, x and $\overline{x}$ represent the Raman intensity and the average value of the samples, respectively; MR represents the moving range, which is $MR = |x_{i+1} - x_i|$; x_i represents the Raman intensity of the sample i variable, and i changes from 1 to 29 in steps of 1 in this work. UCL = upper control limit; LCL = lower control limit; $\overline{MR}$ = the average value of moving range control chart.
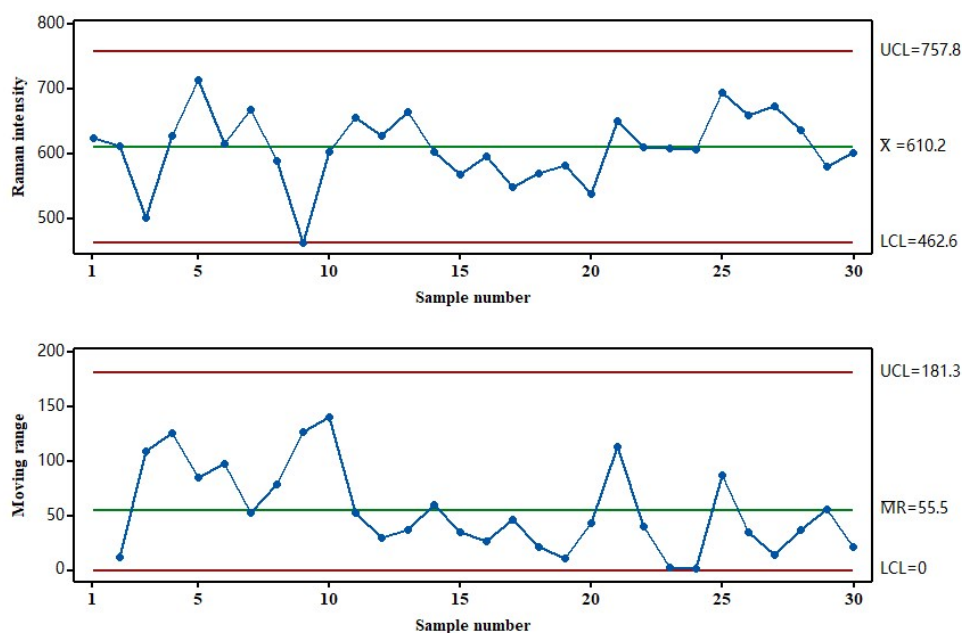
Figure S5 Quality fluctuation individual value chart (A) and moving range chart (B) of MS based on Raman peak intensities (at 1468 cm⁻¹).
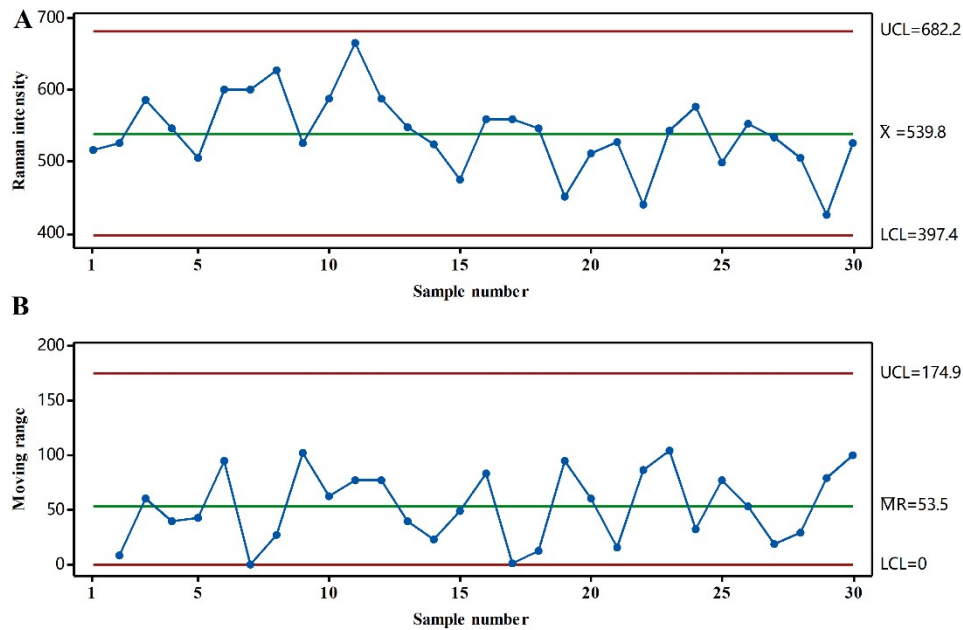
Figure S6 Quality fluctuation individual value chart (A) and moving range chart (B) of AM based on Raman peak intensities (at 1468 cm^{-1}).

(UCL represents upper control limit; LCL represents lower control limit; $\overline{MR}$ represents the average value of moving range control chart. AM represents the ambpoeial pasteurized heat-treated flavor yoghurt products from Inner Mongolia Yili Industrial Group Co., Ltd.)
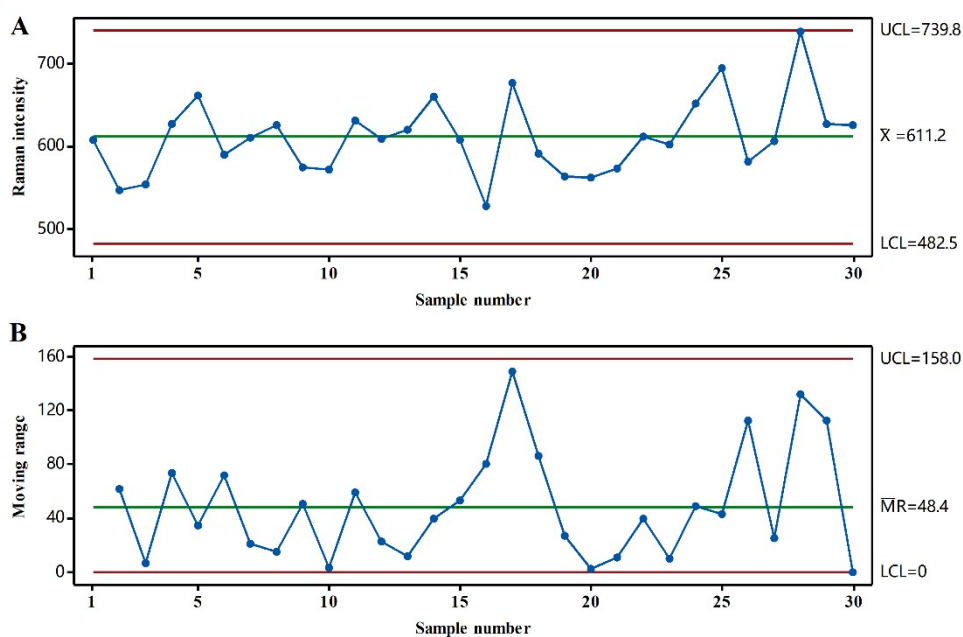
Figure S7 Quality fluctuation individual value chart (A) and moving range chart (B) of CZ based on Raman peak intensities (at 1468 cm^{-1}).

(UCL represents upper control limit; LCL represents lower control limit; $\overline{MR}$ represents the average value of moving range control chart. CZ represents the ChunZhen pasteurized heat-treated flavor yoghurt products from Mengniu Dairy Group Co. Ltd.)

Table S1 Composition content of dairy products

Chemical composition	MS	AM	CZ
Protein	2.8g/100g	3.1g/100g	2.8g/100g
Fat	3.0g/100g	3.1g/100g	3.2g/100g
Sugar	12.5g/100g	13.0g/100g	12.5g/100g

(MS represents the momchilovtsi pasteurized heat-treated flavor yoghurt products from Bright Dairy & Food Co., Ltd. AM represents the ambpoeial pasteurized heat-treated flavor yoghurt products from Inner Mongolia Yili Industrial Group Co., Ltd. CZ represents the ChunZhen pasteurized heat-treated flavor yoghurt products from Mengniu Dairy Group Co. Ltd.)

Table S2 The identification results of dairy products based on their Raman spectroscopy and SVM recognition algorithm (window interval 20 cm^{-1}).

The range of Raman spectroscopy (cm^{-1})	Accuracy rate (%)	The range of Raman spectroscopy (cm^{-1})	Accuracy rate (%)
255-274	42	1115-1134	48
275-294	57	1135-1154	49
295-314	46	1155-1174	44
315-334	47	1175-1194	55
335-354	56	1195-1214	54
355-374	39	1215-1234	46
375-394	36	1235-1254	54
395-414	43	1255-1274	44
415-434	48	1275-1294	46
435-454	54	1295-1314	64
455-474	46	1315-1334	53
475-494	44	1335-1354	41
495-514	52	1355-1374	43
515-534	55	1375-1394	43
535-554	44	1395-1414	37
555-574	35	1415-1434	49
575-594	42	1435-1454	47
595-614	50	1455-1474	51
615-634	55	1475-1494	49
635-654	62	1495-1514	58
655-674	42	1515-1534	58
675-694	54	1535-1554	50
695-714	56	1555-1574	52
715-734	42	1575-1594	66
735-754	50	1595-1614	53
755-774	57	1615-1634	58
775-794	51	1635-1654	56
795-814	47	1655-1674	49
815-834	58	1675-1694	49
835-854	47	1695-1714	56
855-874	43	1715-1734	47
875-894	45	1735-1754	53
895-914	52	**1755-1774**	**69**
915-934	50	1775-1794	43
935-954	47	1795-1814	60
955-974	49	1815-1834	54
975-994	50	1835-1854	63
995-1014	47	1855-1874	60

1015-1034	62	1875-1894	60
1035-1054	57	1895-1914	60
1055-1074	48	1915-1934	56
1075-1094	37	1935-1954	57
1095-1114	51	1955-1974	55

Table S3 The identification results of dairy products based on their Raman spectroscopy and SVM recognition algorithm (Raman band scanning).

The range of Raman spectroscopy (cm^{-1})	Accuracy rate (%)	The range of Raman spectroscopy (cm^{-1})	Accuracy rate (%)
350-405	35	1155-1185	51
485-540	61	1185-1230	50
590-670	47	1230-1300	52
780-820	52	1300-1415	59
820-915	57	1415-1520	55
915-985	44	1550-1580	55
985-1030	56	1580-1605	62
1030-1060	53	1605-1640	59
1060-1115	41	1640-1730	49
1115-1155	41	1730-1800	57
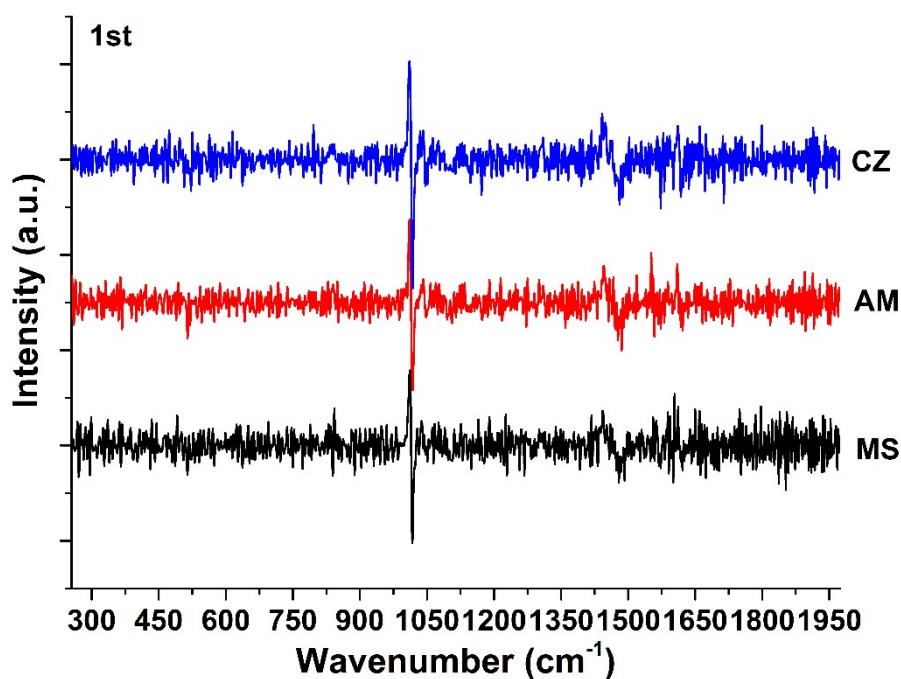
Figure S8 Raman spectra of different dairy products after first order derivative

processing.

(MS represents the momchilovtsi pasteurized heat-treated flavor yoghurt products from Bright Dairy & Food Co., Ltd. AM represents the ambpoeial pasteurized heat-treated flavor yoghurt products from Inner Mongolia Yili Industrial Group Co., Ltd. CZ represents the ChunZhen pasteurized heat-treated flavor yoghurt products from Mengniu Dairy Group Co. Ltd.)
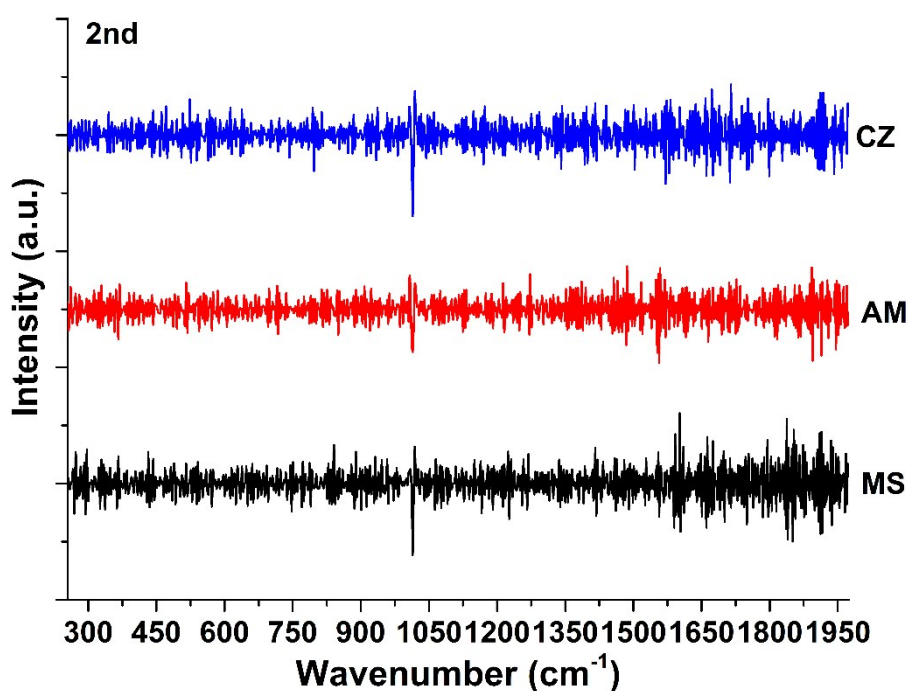
Figure S9 Raman spectra of different dairy products after second order derivative processing.
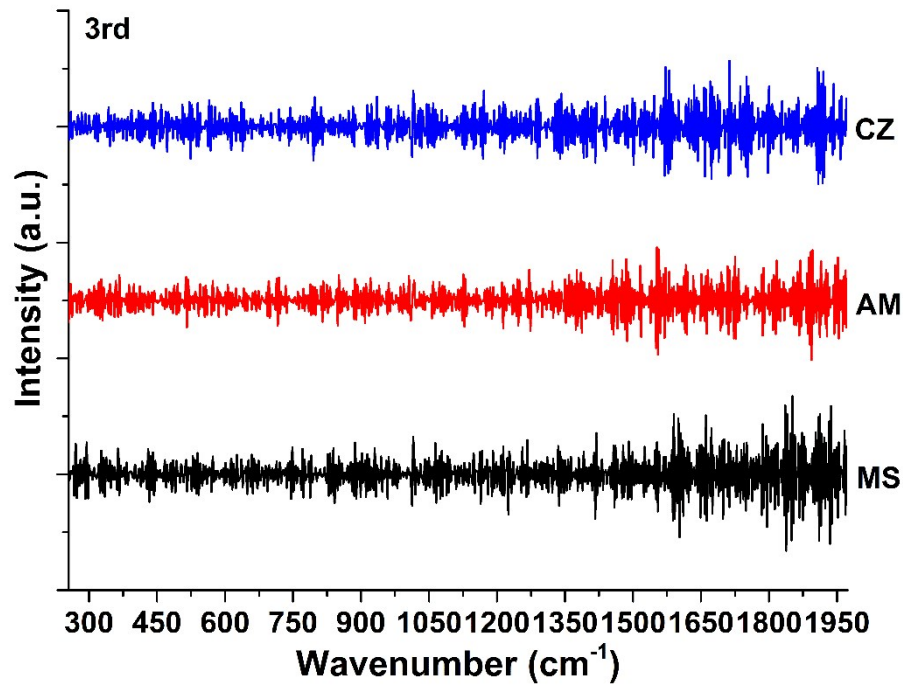
(MS represents the momchilovtsi pasteurized heat-treated flavor yoghurt products from Bright Dairy & Food Co., Ltd. AM represents the ambpoeial pasteurized heat-treated flavor yoghurt products from Inner Mongolia Yili Industrial Group Co., Ltd. CZ represents the ChunZhen pasteurized heat-treated flavor yoghurt products from Mengniu Dairy Group Co. Ltd.)

Figure S10 Raman spectra of different dairy products after third order derivative processing.
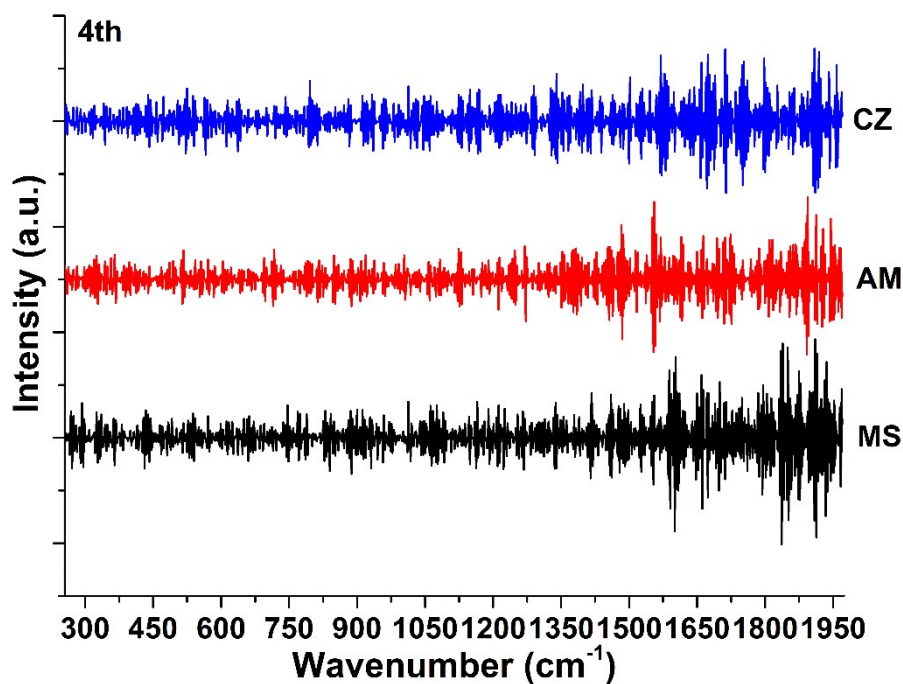
(MS represents the momchilovtsi pasteurized heat-treated flavor yoghurt products from Bright Dairy & Food Co., Ltd. AM represents the ambpoeial pasteurized heat-treated flavor yoghurt products from Inner Mongolia Yili Industrial Group Co., Ltd. CZ represents the ChunZhen pasteurized heat-treated flavor yoghurt products from Mengniu Dairy Group Co. Ltd.)

Figure S11 Raman spectra of different dairy products after fourth order derivative processing.

(MS represents the momchilovtsi pasteurized heat-treated flavor yoghurt products from Bright Dairy & Food Co., Ltd. AM represents the ambpoeial pasteurized heat-treated flavor yoghurt products from Inner Mongolia Yili Industrial Group Co., Ltd. CZ represents the ChunZhen pasteurized heat-treated flavor yoghurt products from Mengniu Dairy Group Co. Ltd.)
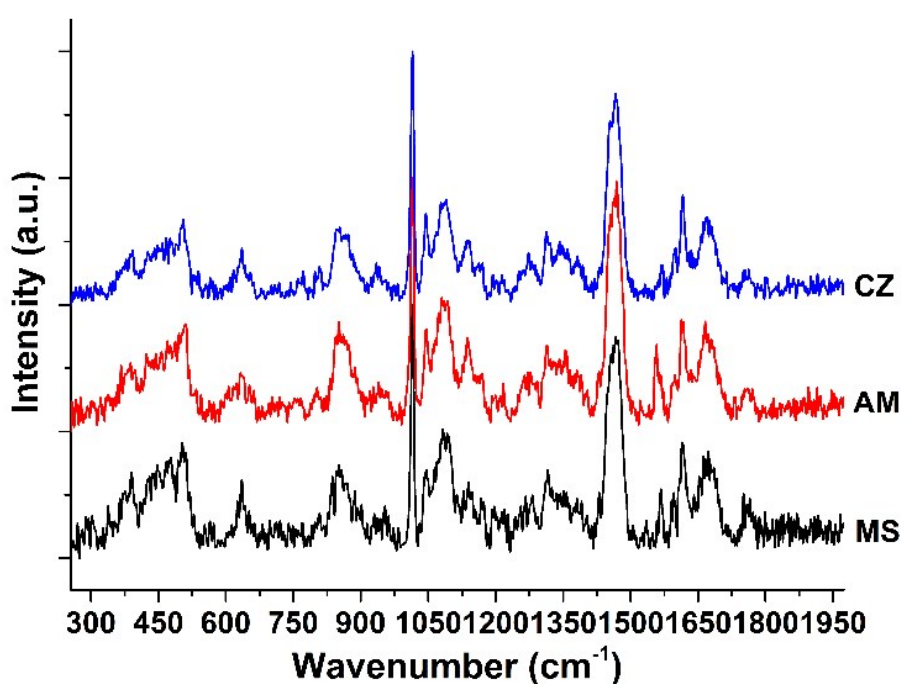

Figure S12 Raman spectra of different dairy products after normalization.

(MS represents the momchilovtsi pasteurized heat-treated flavor yoghurt products from Bright Dairy & Food Co., Ltd. AM represents the ambpoeial pasteurized heat-treated flavor yoghurt products from Inner Mongolia Yili Industrial Group Co., Ltd. CZ represents the ChunZhen pasteurized heat-treated flavor yoghurt products from Mengniu Dairy Group Co. Ltd.)

Table S4 The identification results of dairy products based on their Raman spectroscopy and SVM recognition algorithm after normalization (window interval 20 cm^{-1}).

The range of Raman spectroscopy (cm^{-1})	Accuracy rate (%)	The range of Raman spectroscopy (cm^{-1})	Accuracy rate (%)
255-274	44	1115-1134	61
275-294	57	1135-1154	60
295-314	53	1155-1174	57
315-334	48	1175-1194	55
335-354	**71**	1195-1214	53
355-374	51	1215-1234	41
375-394	53	1235-1254	57
395-414	57	1255-1274	50
415-434	55	1275-1294	60
435-454	**71**	1295-1314	55
455-474	61	1315-1334	60
475-494	65	1335-1354	53
495-514	57	1355-1374	51
515-534	65	1375-1394	51
535-554	48	1395-1414	53
555-574	46	1415-1434	62
575-594	46	1435-1454	62
595-614	52	1455-1474	59
615-634	61	1475-1494	57
635-654	64	1495-1514	57
655-674	42	1515-1534	53
675-694	40	1535-1554	53
695-714	55	1555-1574	69
715-734	45	1575-1594	58
735-754	51	1595-1614	58
755-774	50	1615-1634	64
775-794	55	1635-1654	60
795-814	43	1655-1674	58
815-834	59	1675-1694	63
835-854	**75**	1695-1714	59
855-874	57	1715-1734	48
875-894	51	1735-1754	61
895-914	49	1755-1774	65
915-934	54	1775-1794	49
935-954	53	1795-1814	51
955-974	50	1815-1834	49
975-994	47	1835-1854	49

995-1014	54	1855-1874	51
1015-1034	53	1875-1894	63
1035-1054	54	1895-1914	60
1055-1074	53	1915-1934	50
1075-1094	52	1935-1954	50
1095-1114	56	1955-1974	50

Table S5 The identification results of dairy products based on their Raman spectroscopy and SVM recognition algorithm after normalization (Raman band scanning).

The range of Raman spectroscopy (cm^{-1})	Accuracy rate (%)	The range of Raman spectroscopy (cm^{-1})	Accuracy rate (%)
350-405	60	**1155-1185**	**70**
485-540	**72**	1185-1230	56
590-670	66	1230-1300	65
780-820	61	**1300-1415**	**71**
820-915	**83**	1415-1520	73
915-985	62	1550-1580	61
985-1030	58	1580-1605	59
1030-1060	61	1605-1640	65
1060-1115	61	1640-1730	63
1115-1155	68	1730-1800	60

References

1 D.C. Montgomery, *Introduction to Statistical Quality Control (Sixth Edition)*, John Wiley & Sons, Inc., 2009.