Supporting Information

A novel strategy to identify analytical markers of Cerebralcare Granule for quality assessment by ultra-high performance chromatography and chemometric analysis

Contents

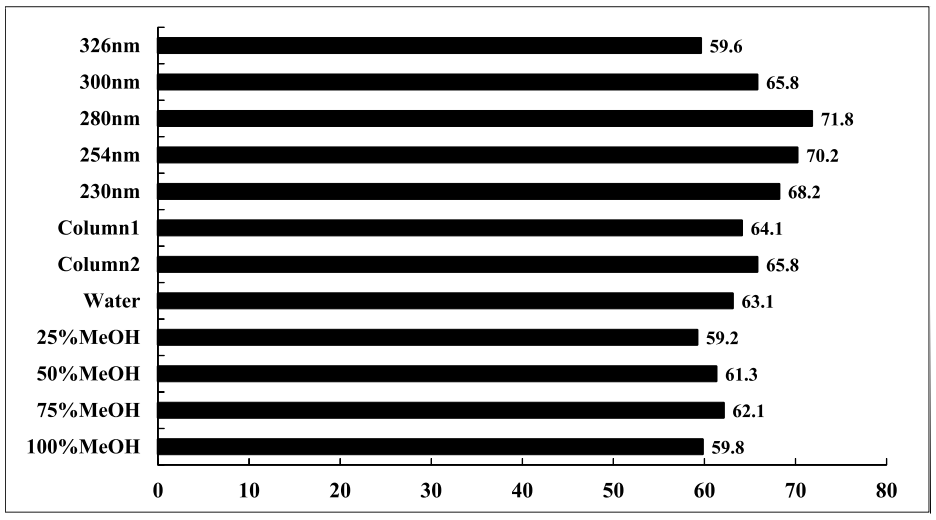

Figure. S1 The *Ir* value under different condition (extraction solvents, detection wavelength, extraction method, column). The index of the fingerprint information amount (*Ir*) was adopted to screen the optimized condition for sample extraction and separation and *Ir* was the index which represents the signal size, signal homogenization and the information amount.

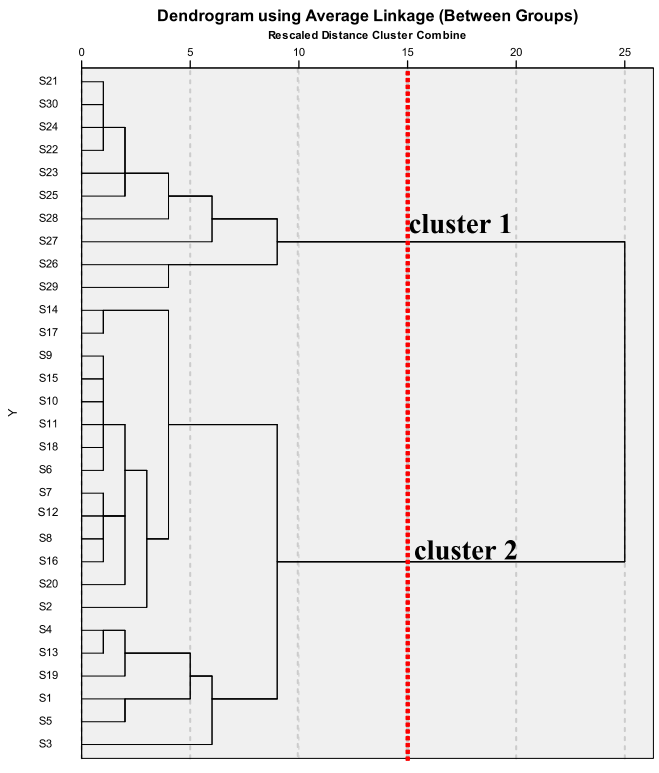

Figure.S2 Hierarchical Cluster Analysis: dendrogram based on Euclidean distance of 30 batches of CG samples. Samples S01-S20 were in cluster 1; samples S21-S30 in cluster 2.

Table.S1 A summary of the investigated CG samples.

Sample	Brand	Date of manufacture	Date of expiration	Date of analysis	Type
S1	Tasly	2013.05	2016.05	2014.10	Qualified
S2	Tasly	2013.06	2016.06	2014.10	Qualified
S3	Tasly	2013.05	2016.05	2014.10	Qualified
S4	Tasly	2013.05	2016.05	2014.10	Qualified
S5	Tasly	2013.06	2016.06	2014.10	Qualified
S6	Tasly	2013.06	2016.06	2014.10	Qualified
S7	Tasly	2013.11	2016.11	2014.10	Qualified
S8	Tasly	2013.10	2016.10	2014.10	Qualified
S9	Tasly	2013.05	2016.05	2014.10	Qualified
S10	Tasly	2013.05	2016.05	2014.10	Qualified
S11	Tasly	2013.05	2016.05	2014.10	Qualified
S12	Tasly	2013.05	2016.05	2014.10	Qualified
S13	Tasly	2013.05	2016.05	2014.10	Qualified
S14	Tasly	2013.05	2016.05	2014.10	Qualified
S15	Tasly	2013.04	2016.04	2014.10	Qualified
S16	Tasly	2013.05	2016.05	2014.10	Qualified
S17	Tasly	2013.05	2016.05	2014.10	Qualified
S18	Tasly	2013.05	2016.05	2014.10	Qualified
S19	Tasly	2013.05	2016.05	2014.10	Qualified
S20	Tasly	2013.05	2016.05	2014.10	Qualified
S21	Tasly	2009.12	2013.12	2014.10	Expired
S22	Tasly	2009.12	2013.12	2014.10	Expired
S23	Tasly	2009.06	2013.06	2014.10	Expired
S24	Tasly	2009.06	2013.06	2014.10	Expired
S25	Tasly	2009.07	2013.07	2014.10	Expired
S26	Tasly	2009.12	2013.12	2014.10	Expired
S27	Tasly	2010.01	2014.01	2014.10	Expired
S28	Tasly	2009.08	2013.08	2014.10	Expired
S29	Tasly	2009.11	2013.11	2014.10	Expired
S30	Tasly	2009.12	2013.12	2014.10	Expired

Table.S2 The quality grade assigned by SQFM and the acceptance criteria

Qualitity grade	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
$S_m \geq$	0.95	0.90	0.85	0.80	0.70	0.60	0.50	$S_m \leq 0.50$
$P_m \in$	95～105	90～110	80～120	75～125	70～130	60～140	50～150	0～∞
$\alpha \leq$	0.05	0.10	0.15	0.20	0.30	0.40	0.50	＞0.50
Quality	Best	Better	Good	Fine	Moderate	Common	Defective	Inferior

Table.S3 The similarity analysis results obtained using.

Parameter	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11
S_m	0.73	0.88	0.81	0.80	0.82	0.92	0.92	0.89	0.91	0.90	0.90
P_m	99.70	87.00	96.40	105.50	98.10	87.90	100.30	106.90	94.00	95.60	93.00
α	0.00	0.06	0.09	0.00	0.04	0.03	0.04	0.03	0.02	0.03	0.00
Grade	4	3	4	4	4	3	2	3	2	3	3
Parameter	S12	S13	S14	S15	S16	S17	S18	S19	S20	S21	S22
S_m	0.91	0.84	0.92	0.92	0.89	0.92	0.90	0.81	0.86	0.80	0.78
P_m	100.50	106.20	109.40	93.20	103.20	106.20	96.80	104.40	98.80	124.50	119.90
α	0.05	0.01	0.06	0.03	0.02	0.07	0.01	0.04	0.03	0.14	0.12
Grade	2	4	2	2	3	2	2	4	3	5	5
Parameter	S23	S24	S25	S26	S27	S28	S29	S30	RFP	Average	RSD (%)
S_m	0.77	0.78	0.82	0.67	0.79	0.79	0.68	0.79	1	0.08	9.39
P_m	129.60	120.80	130.60	134.90	106.80	126.20	119.50	123.70	100	13.35	12.47
α	0.13	0.14	0.15	0.15	0.17	0.20	0.13	0.14	0	0.06	84.83
Grade	5	5	6	6	5	5	6	5	1	--	--

Table.S4 The data matrix of similarity calculation.

No	G[a]1	G2	G3	G4	G5	G6	G7	G8	G9	G10	G11
S[b]1	60384.7	249382.8	163386.8	187693.3	75629.5	511672.7	231473	133186.9	196497.1	94613.1	27879.1
S2	43724.8	161674.2	137016.1	124021.3	90605.2	546964	173537.1	154422.9	239596.7	148451	35685.9
S3	73381.1	83965.2	130192.5	275080.1	161687.1	616737.3	247226.4	129084.8	227201.5	109235.7	30509.6
S4	97635.9	254627.1	216220	235141.3	124897.8	531728	354669.2	122816.3	217435.5	113916.4	28318.4
S5	96413	172884.1	277593.9	325757.7	190089	582789.3	321810	135536.4	292586.9	128400.5	33995.6
S6	79251.3	137796.7	243486.7	270882.7	169104.4	530975.4	289275.7	106239.3	247053.1	119384.9	32575.7
S7	48932.3	175653.9	218920	245243.4	143942.8	547900.2	245864.8	101379.3	227663.5	115738.5	32513.8
S8	33409.1	204356.6	219879.5	285317.2	264993.4	563014.8	167803.7	124812.2	145995.7	73662.6	29871.8
S9	58705.6	161194.4	242762.4	259814.2	156318.2	532032.8	319862.5	125532.5	209186.8	116938	36246.4
S10	52248	138833.1	245206.8	262938.3	56.3	540774.3	157911	128081.6	222836.4	115109	33986.2
S11	49924.1	198768.3	172035.3	100291	179913.9	548123.3	309408	119640.3	247132.2	139727.1	37894.4
S12	58235.5	178109.1	168093.1	115268	170938.1	561144.5	324137.1	96868.2	215974.8	108418.5	1025.2
S13	44238.6	172439.5	113317.9	147674.2	49586.2	554024.1	315347.1	139945.2	246432.8	115931.8	214.5
S14	36863	309672.5	141338.4	107721.9	178860.8	581469.3	326274.6	151867.3	192579.8	106253.4	5478.2
S15	35840.1	226124.7	492847.8	6969.775	188926.4	603140	309316.4	137984.8	183012	150262	4521.2
S16	57754.4	195965.3	524030.6	8921.475	90979.6	598262.3	344170.3	134976.1	241908	113355.6	2541.2
S17	50055.2	298246.7	456037.9	7627.4	147487.9	609107	360567.9	157017.4	179152.9	110403	2515.3
S18	84542.2	371811.7	645189	7079.6	91682.4	614454.2	221583.1	122673.3	275145.3	126793.7	3512.8
S19	100427.5	220496	534304.4	8498.9	229686.8	622069.5	355927.6	144327.1	271464.5	128867.1	1101.2
S20	53000.2	134417.5	552601.2	8143.925	41799	569597.1	343071.8	148084.3	233902.6	100959.1	112.3
S21	33830	334751.9	490464.1	7467.95	321.3	553532.2	285637.8	94543.7	265439.9	218329.7	26419.4
S22	38906.5	191212.8	400539.9	9061.6	90016.8	536043.5	270054.4	122992.3	229963.3	224434.5	15237.6
S23	78379.7	202254.8	458629.8	1393.955	128770.4	554281.3	296766.9	92724.8	281888.9	295710.5	222.5
S24	78979.6	203802.9	379626.5	1784.295	46270	558523.9	299038.4	93434.5	284046.6	297973.9	1873
S25	52374.2	228104.6	450500.9	1525.48	123204.3	530993.4	308416.1	123152.3	339369.6	373504.4	33633.5
S26	49681.9	152342.1	532740	1415.92	136456.4	561418.1	344879.8	124884.1	225844.7	246684.4	23653.7
S27	33259.3	169866.5	398817.7	1699.78	152740.3	453662.6	229382.5	77738.4	146022.9	171606	35763.6
S28	94909.8	379913.3	447907.9	1628.785	65699.5	569645	242820.2	109650.1	269602.9	209766	51520
S29	22944.7	226102.4	431924.2	1625.69	60052.1	532654.9	359835.3	133735.5	224727.2	212325	55142.5
S30	38510.2	122236	418250.2	1493.59	150381.2	519856	12756	90721	200170.5	170706.3	42428.8

No	G12	G13	G14	G15	G16	G17	G18	G19	G20	G21	G22
S1	46985.4	83038.8	226784	153804.6	121669.1	135615.6	74323.8	193828.5	261207.3	49154.2	240691.7
S2	51336.4	134549.3	390038.8	155060	180432.5	160582	74999.8	206611	267624.6	46736.5	300747.1
S3	37286.7	80269	271487	75881.2	123796.2	161320.3	89634.7	244794	280034.3	87952.9	289327.5
S4	39449	131728.5	289199.8	161559.1	147113.5	0	63386.4	174013.8	184340	62897.7	316030.3
S5	1254.2	133881.1	334386.6	127998.3	122863	174934.4	76262.1	229627.2	213637.3	90853.3	404542.9
S6	44446.1	126826.4	300185.1	112509.5	113498.2	0	60500.9	199272.4	201913.3	43489	312493.7
S7	44027.7	127356.3	238813.9	145188.5	123068.7	158476.4	63671.3	179172.9	191803.4	45393.6	320441.4
S8	30044.6	102934.4	288645.6	96339.7	246706.3	172704.6	70649.9	226403.2	230208.5	51802.2	426231.7
S9	41124.9	107218.1	204212.9	143098.8	147209.4	155942.2	59934.4	152284.2	182297.6	73199.4	302945.7
S10	40077.4	109866.1	239648.5	139208.4	155006.7	152078.5	61025	152723.1	177528.7	57292.4	315139.3
S11	66584.1	134529.2	307295.1	148679.8	233943.1	164455.2	72251.9	199737.5	231686.1	85664.6	337369
S12	136063.9	4765.2	397888.5	175669.7	220386.2	175369.7	78275.7	233281.9	270690.9	64867.9	469655.6
S13	139367.2	7895.2	293848.9	161199.2	205374.3	171170.7	62339.4	221503.7	279178.8	48534.2	347969.4
S14	114746.8	3685.1	355445.8	131879.7	211449.8	142983	61559	216019.5	255863.9	54762.2	372685.9
S15	119701.9	1587.2	383055.5	136274.3	226247.3	138137.7	81491.1	229513.2	325352.8	36547.4	379611.6
S16	139516.6	2543.3	334875.2	150444.4	203988.7	143694.9	60995.5	228522.3	259832.2	81684.6	18996.42
S17	115277.8	2589.1	364723.4	137321.3	229694.3	143415.3	60192.1	256228.1	197773	58725.4	13657.07
S18	119980.1	1875.3	363924.8	181096	199211.1	167559.4	64268.1	250215.1	305322.4	66937.4	15566.84
S19	92238.3	3254.2	349614.4	166189.1	358.9	152178.2	60891.5	231846.6	279057.5	122373.1	28458.86
S20	135834	853.4	288484.8	149498.2	2589.4	147163.2	54878	203736.4	251292.4	65724.2	15284.7
S21	129882.9	258.6	665874.8	209487.5	3089.786	148103.1	66763.6	290672.8	484642.7	2744.528	726.0656
S22	116678.9	3587.2	632987.6	285329.5	4208.4	134147.1	67632.5	246046.2	473479.5	2604.338	688.9783
S23	69087.4	4583.1	751871.2	348663.4	5142.528	144174.7	60173.3	177692.9	253.4	2888.729	764.214
S24	75469.9	3586.4	757626.3	351332.2	5181.891	145278.3	61948.4	178658.9	3585.2	2130.217	563.5495
S25	206798.7	589.4	793192.2	414469.6	6113.121	191000.4	65480.4	282149.8	228.68	28643.5	7577.646
S26	107215.6	7893.1	618740.9	268731.3	3963.588	175113.9	73612.8	297100.3	468164	43841.8	11598.36
S27	97806	1893	493407.2	231484.4	214347.9	139036	66900.9	224085.3	384827.9	0	442802.1
S28	90819.1	1896.2	686851.7	306192.3	209243.7	161602	76682.8	259049.6	456550	51209.9	600088.4
S29	82530.7	97132.4	518763.8	231426.1	144410.4	170996.4	81043.7	238743	405752.6	67964.2	465063.7
S30	84545.2	110750.9	549646.1	231122.3	236707.9	163696.2	82132	228190.5	406594.2	68430.3	537562.5

No	G23	G24	G25	G26	G27	G28	G29	G30	G31	G32	G33
S1	57447.1	85209.5	218368	799878.3	39066	673758.9	453595.9	510439.3	2984757	121377	1467171
S2	39350.7	61358.8	225528.8	243801.2	38822.8	656616	418449.6	479788.5	2844435	110718.5	1305742
S3	47280	58952.1	189755.7	279012.9	46537.6	412507.7	147622	479117.2	3042078	113233.3	1673369
S4	23757.8	99996.8	192144.6	394557.2	42635.3	714165.3	598323.6	647200.8	2970440	120656.8	1462789
S5	59650.2	102526	187001.3	131103.9	42577.2	1390480	0	620153.6	3259904	139071	1684003
S6	33251.9	63502.7	206522.5	289521.7	44067.1	660231	648782.1	408117.1	2997900	112620.7	1434019
S7	0	102795.2	206277.2	252452.6	40286.2	658024.2	616052.4	370032	3034993	113270.5	1527467
S8	46782	82544.9	202737.3	357771.1	46290.8	811554.8	687896.2	622873.6	3214879	144978.3	1851041
S9	34744.3	86796.8	198789.1	257982.5	36903.5	677976.3	599718.6	596698.9	3020282	118119.2	1402055
S10	34987.8	76434.9	198029.2	288444.1	35437.3	706284.6	570703.3	587269.5	2977330	95219.6	1397261
S11	35421.7	4834.257	187849.4	657155.1	38115.5	622628.4	584891	559229.8	2802572	110633.1	1350458
S12	39476.8	4195.208	200984.1	1066.918	0	617762.7	1596.5	658.24	3456248	148724.1	1938390
S13	35323.6	3772.061	208180.5	1169.459	81554	628680.6	2586.1	33345.5	3061870	0	1421036
S14	35272.6	4766.383	220606.1	911.2423	77909	694722.7	562753.6	145.2	3456009	0	1863688
S15	37771.2	3205.983	224910.7	1581.732	84300.4	707275.5	471523	2896.1	2536441	0	1324748
S16	37695.6	3215.223	185817	817.2648	66905.6	664410.2	672540.2	610011.3	2958568	127993.9	1594374
S17	35290.7	4205	272001.8	939.0761	77486.2	656876.2	596424.4	573705.7	3648163	126040.2	1775252
S18	38421.4	4911.198	280746.9	882.8986	70598.8	707144.3	625425.1	668418.3	3106929	0	1655674
S19	31040.4	4663.236	568.4	1056.983	96775.4	671503.7	752960.6	664157	456.87	131020.8	1788250
S20	30642.7	4535.2	521.4	1270.47	66689.3	637203.4	595550.1	536893.4	358.47	124327.2	1454840
S21	0	12209.54	1112.434	1066.918	92297.9	521200.2	629439.8	736696.2	1278.964	200946.3	2635548
S22	25011.3	12430.15	1299.259	1169.459	91004.5	567345.7	515959	626688.9	1753.178	175612.9	2295586
S23	0	11676.8	1233.66	911.2423	70170.5	549862.1	1586.1	702162.5	1208.139	173768.8	28159.4
S24	156.5	11544.4	1203.116	1581.732	70707.6	554070.9	3873.2	707537.1	1038.817	175098.9	23446.4
S25	28358.2	12427.84	1278.269	817.2648	91681.8	982224.4	0	752415.1	1672.063	195773.2	55210.9
S26	158.38	11801.47	0	939.0761	0	622871.1	619943.6	497169.1	1352.8	186922	2550551
S27	532.14	11198.65	229798.9	882.8986	77348.3	543908.3	402124.2	0	4196732	148236.1	2149864
S28	1693	12421.53	296556.1	365.4	0	1216811	531179	0	5322178	202360.4	2773221
S29	106303.7	9159.933	265417.3	457442	85173.7	1029162	634607	608075.3	4733977	169830.5	2262848
S30	2873.1	386.4	244863.6	874475.1	38906.5	1011611	490734.7	507601	4375839	173582.7	2278229

No	G34	G35	G36	G37	G38	G39	G40	G41	G42	G43	G44
S1	31250.2	669315.9	55417.3	45811.4	271450.6	142249.7	28038.6	330177	63382.9	234554.7	172465.5
S2	49339.3	636833.1	42622.4	27745.7	213926.7	113126.8	24297.4	322175.5	44987.9	220133.9	163483.5
S3	63929.3	721263.2	82786	36104	227142.3	243360.6	286.4	327518.5	45668.9	334466.2	0

S4	63907.7	646101	83456.5	48209.5	248953.2	226509.5	19502.2	268721.7	43963	216952.2	139725.1
S5	55385.3	694981.4	157753.7	37875.6	223614.6	224645.9	4091.911	333480.7	57688.7	263594.8	167054.7
S6	28100.4	694152	44584.3	41515.8	232406.4	128781.3	2345.743	333842	54327.4	229577.7	165094.3
S7	26515.7	758912.4	40421.9	32349.1	222516	132272.6	2409.337	383771.4	57226.8	107979.1	38077.2
S8	59647.9	886172.1	65458.4	56151.5	293153	164041.5	2988.005	257514.6	69132.8	179432.6	142293.3
S9	74783.2	649821.2	77673.3	29012.9	212150.6	210248.9	3829.67	294798.1	37393.2	249405	166238.2
S10	65036.7	587367.6	76114.7	33337.2	206569.4	201643	3672.914	275664.9	69872.4	241129.6	119955.3
S11	47359	592965.2	166517.8	31342.9	194282.7	187572.2	3416.616	275515	41920.2	214497.8	138120.5
S12	59182.4	861064.3	159062.2	37522.9	241905.3	156541	2851.384	316001.7	68209.1	242605.8	176944.9
S13	59742.4	815921.4	162321.7	45101.7	254903.9	188294.3	3429.769	276575.9	65813.3	354086.9	0
S14	78962.2	966799.1	120025.4	301766.6	3996.909	229070.9	229.3	340248.7	121683.1	400406.9	0
S15	45739.5	778424.5	110370.5	47686	631.6026	147102.3	39217.1	235680.2	77678	172724.4	140147.7
S16	56302.5	686238.5	172225.5	218955.1	2900.068	230069.9	0	230304.3	73641.2	353297	3661.109
S17	54773.6	855066	137407.3	269386.9	3568.038	208100.1	35561.4	314654.1	69431	385298.6	3992.732
S18	739132.7	26233.9	167924.5	227973.1	3019.511	212141.5	2424.474	253517.6	0	363717	3769.088
S19	772866.7	23697.7	225996.9	281715.6	3731.332	277369.4	3169.936	295854.7	92298.4	375369.8	3889.842
S20	695756.3	30487.5	149569.9	206995.6	2741.664	200810	2294.971	232429.7	68081	316081.7	3275.458
S21	1122591	11633.07	162602.7	331391.7	8607.577	123231.4	62696.5	470769.7	103227.9	718395.9	7444.517
S22	1133904	11750.3	110909.5	283508.2	7363.849	133387.2	50545.4	499383.7	131657.8	683214.2	17745.82
S23	1130480	11714.81	171918.3	298359.1	7749.587	53688.8	46525.2	440327.2	108352.4	741912.1	19270.44
S24	1139133	11804.48	173234.3	300642.9	7808.906	54099.7	46881.3	443697.6	109181.8	747591	19417.95
S25	1288230	13349.54	146392.4	331845.6	8619.366	61022.7	60197.3	527893.5	103786.1	825676.5	21446.14
S26	1058238	10966.2	159260.7	304449.4	7907.777	130342.3	53542.3	433816.5	102374.7	682511.8	17727.58
S27	39362.1	1000271	100508.3	47725.1	1239.613	83230.2	58325.5	447120.5	85588.4	308281.4	8007.309
S28	44842.5	1181746	0	84151.1	372690.1	120360.9	146561.8	793855	196212.1	591114.1	15353.61
S29	60124.6	947145.5	59388.7	0	289032.1	133859.4	0	464823.2	95523.6	353630.4	284131.4
S30	32328.1	932482.6	98215	45253	249315.8	110071.1	57154.9	481205.2	0	329198.1	288714.4

No	G45	G46	G47	G48	G49	G50	G51	G52	G53	G54	G55
S1	91693.1	22910.8	16667.3	52980.4	18879.4	707726.5	153136	34449.3	12142.1	33098.3	381066
S2	76910.3	21115.1	15256.8	375.2	0	458754	74690.3	29981.9	97.5	763.2	296913.9
S3	88160.6	19464.2	15179.3	679.2	18776.8	595431.1	122221.2	40957.3	39.5	34674.1	377689.5
S4	85594.3	21509.9	14222.7	45725.8	23454.8	829036.8	148303.5	50177.1	17478.1	33924.1	471606.9
S5	94346.7	23466.7	21504.7	54521.8	19906.6	645224.5	128328	36612.4	256.1	33550	392249.4
S6	85520.5	21539.2	16336.6	185.6	21449.6	602064.2	112136.6	36334.7	123.4	689.4	430839.5
S7	37789.2	21875.9	10982.3	51325.1	32036.1	666619.5	147966.4	31799.6	289.4	896.5	454429.9
S8	99176.5	22358.1	18238.3	50482.9	23962.3	746347.2	115275.8	53096	357.1	37308.9	519400.7
S9	82552.5	21393.2	15885.9	135.2	20323.1	689054.5	138225.7	38564.5	197.5	26108	377155.3
S10	50532.8	17645.5	12484.1	23947.8	13565.1	605324.7	120898.2	40086.4	153.8	21971.6	418957.3
S11	95753.9	15192.4	15681.5	31725.6	18908.4	653836.6	123669.3	37201.7	368.4	31177.7	377962
S12	76776.6	19463.2	31943.3	63181.8	0	705600.1	136863.6	42592.5	178.9	31958.9	479087.6
S13	71882.5	22158.2	23300.7	43341.3	15567.4	914572.5	163720.4	54409.3	35515.1	55892.3	576024.6
S14	82854.8	23950.3	27954.5	46384.6	24494.4	828818.5	155283.9	51076.7	538.4	54317.2	573838.2
S15	79375.2	37374.4	23306.1	39980.4	19854	746551.3	97746.4	51661.8	19799.5	30613.7	550518.6
S16	58686.3	26233.9	22963.8	22380.8	1406.17	596369.1	113414.3	38605.4	863.4	44949.6	394974.4
S17	51387.2	23697.7	28023.9	27440.9	1345.484	807018.5	148171.1	48657.7	18151.2	35792.5	556153.1
S18	70547.6	30487.5	22843.4	22260.4	1109.78	688284.3	133323	42682.7	189.5	77884.9	461884.3
S19	86517	28648.5	22170.4	46730.7	955.4969	868938.9	160623.3	56230.1	15662.7	41193.4	545625.3
S20	59652.2	28159.4	19140.6	33095.1	1224.101	634724.6	119177.9	41376.4	368.7	35251.9	435861.6
S21	120270.1	55210.9	30643.1	33579.3	0	768227.1	224789.5	41801.1	27989.7	49164.7	406072.6
S22	90423.7	45952.3	37444.1	372.5	0	642981.1	164187.5	36018.4	32833.1	189.5	357332.1
S23	152066.6	55571.7	28458.7	46130.9	21340.2	605716	257214.3	36175.6	26405.3	387	317626.4
S24	153230.5	55997.1	28676.6	224.8	0	610352.3	237592.5	36452.5	26607.5	19636.5	320057.6
S25	141535.7	60737.1	30333.2	50133.2	0	609554.2	164888.1	31350.9	18844.4	28730.4	362368.7
S26	96395.7	53526.4	27567.3	179.2	30301.2	589460.1	187424	32731.1	223.1	49472.4	342872
S27	53462.3	17627.3	18818.7	62036.8	14350.5	534662.8	102933	30005.5	9770.8	14173.6	324361.9
S28	118175.8	28257.7	26422.5	71689.2	62261.2	447429.6	150565	68301	198.5	258.2	302466.1
S29	112732.9	31527.4	19625.6	67702	38311.6	780327.1	161328.8	44230.5	21084.7	56508.3	421486.8
S30	118454.8	26969.4	21669.1	58757.1	31137.8	544625.5	146507.5	31597.5	12.8	168.2	315309.7

No	G56	G57	G58	G59	G60	G61	G62	G63	G64
S1	327775.2	202945.3	24436.5	22012.4	571705.6	123302.2	88129.8	61201.1	24632.1
S2	228035.1	120069.3	458.5	689.1	136533.8	38316.3	23715.2	12036.2	369.5
S3	288424.6	98279.3	13034.5	736.5	179499.1	10835	387.5	465.8	258.6
S4	485349.7	236641.9	27440	18621.6	977764.3	81747.9	47575.8	28316.5	654.8
S5	431698.2	128022.7	27966.3	4077.313	511388.7	27863.9	389.4	258.6	257.6
S6	416311.7	133272.2	26137.6	4806.063	589030.7	30777.7	756.8	365.7	4542.4
S7	259049.1	203079.8	3987.5	5557.281	789553.3	49692	24711.7	18176.1	25.1

S8	454677.2	182338	32934.1	2485.563	691592.5	35949.6	478.5	6227.4	5067.1
S9	431412.3	173475.5	32157.5	2504.586	669668.8	58542.2	15962.9	7008.4	9118.5
S10	425527.8	151191.4	32391.5	2227.063	690049.1	32505.1	5467.7	4843	5165.3
S11	398876.8	152592.2	30276.5	2855.422	618388.9	39604.8	4612.4	4992.1	7043.7
S12	508381	200783.6	42122.6	1934.039	923415	49936.8	18681.6	13945.7	7253.8
S13	498164.8	268243.4	41710.4	834.3281	987394.7	106724.2	56196.3	36936.8	15994.4
S14	449064.8	207955	40118.3	14995.4	883580.1	47791.1	15575	9854.7	8259.5
S15	456264.4	226035.6	38413.2	14167.3	816964.4	66389	30009.6	21742.6	5949
S16	397323.3	149305.2	34881.5	687.5	637259.9	37606.8	4058	2764.9	7569.3
S17	476359.5	202928.2	36526.3	14698.9	787902.7	52750.7	23271	16717	7247.7
S18	269670.9	154688.6	789.2	12113.7	651329.4	39388.6	4617.4	4987.8	7235.5
S19	525021.1	255674.7	41522.2	186.4	1065012	81375.1	40057.1	36612.4	16430.5
S20	422001.4	148998.2	25503.7	398.7	648391.2	30484.8	2253.1	3578.3	5412
S21	622673.2	227487.2	39933.2	20806.9	1112136	61517.6	69724.1	49089.7	156.8
S22	472041.9	186800.9	36618.1	3293.93	928675.5	71133.2	69532.8	59133.2	23.5
S23	460140	127886.8	29515.5	3324.449	688995.8	31815.2	18463.6	10709.4	289.2
S24	433310.2	128865.7	29312.5	4374.37	687539.3	32058.7	18604.9	10791.4	5070.4
S25	516368.7	135854.1	37825.1	5844.083	925128.2	28506.4	18532.9	13113.6	147.8
S26	473976.4	152124.5	32688.1	4530.61	881471.5	36549.4	11522.9	8328.5	5965
S27	370192.8	133197.8	30530.5	4924.523	748037	24755.7	34398.7	23248.2	136.5
S28	390511.5	62670.2	26907.8	3252.837	738634.5	10679.4	4833.8	5595.8	478.3
S29	554434.9	222354	21273.5	4421.094	1096619	45702.8	38300.5	32963.9	785.2
S30	417154.1	131450.1	32443.5	3370.122	806566.8	29865.9	14391.5	6920.8	3932.9

a: G represent chromatographic peak number;

b: S represent sample number.

30×64 data matrix, 30 was the number of the samples; each row represented a CG sample and each column contained the values of 64 characteristic peak areas.