Electronic Supplementary Material (ESI) for Molecular BioSystems.

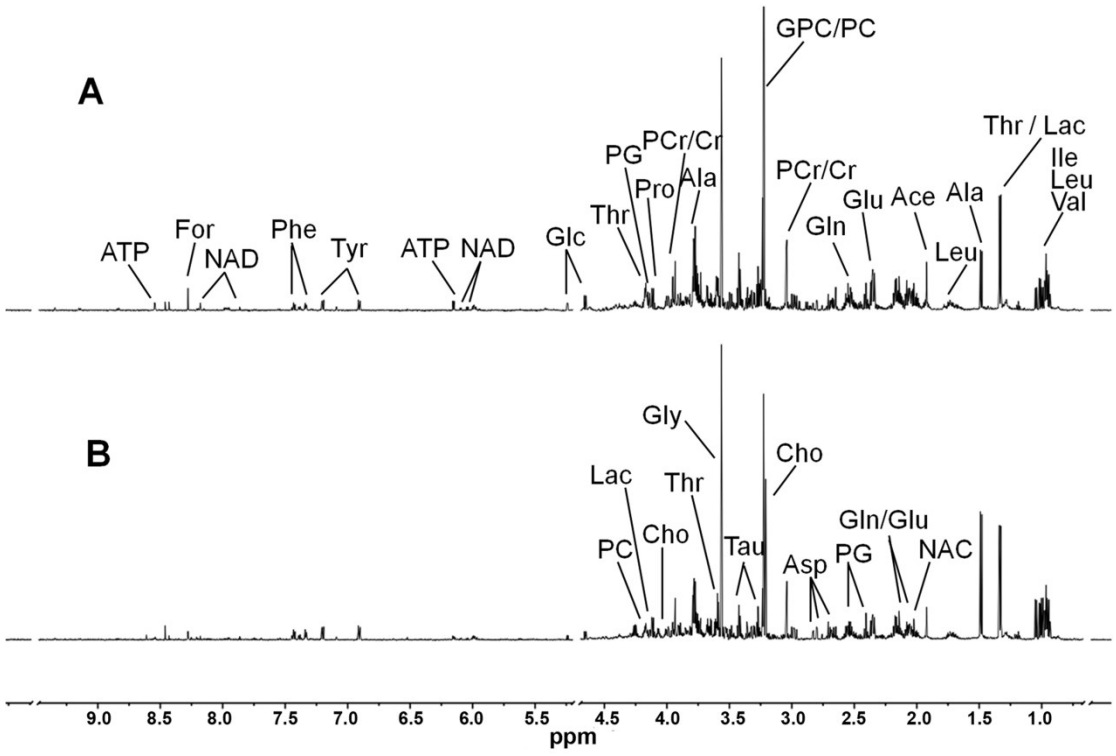

Fig. S1 Representative ^{1}H NMR spectra of aqueous extracts from SGC7901 cells originally cultured in either RPMI1640 (A) or DMEM (B).

Table S1 Components contained in DMEM and RPMI1640.

Components	DMEM (mg/L)	RPMI1640 (mg/L)	Components	DMEM (mg/L)	RPMI1640 (mg/L)
Glucose	4500.00	2000.00	$MgSO_4$	97.67	48.84
Glutamine	584.00	300.00	Folic Acid	4.00	1.00
Riboflavin	0.40	0.20	Inositol	7.20	35.00
Thiamine	4.00	1.00	Choline Chloride	4.00	3.00
Cystine	63.00	65.15	$NaHCO_3$	3700.00	2000.00
Arginine	84.00	290.00	Pyridoxal	4.00	—
Glycine	30.00	10.00	$CaCl_2$	265.00	—
Histidine	42.00	15.00	$Fe(NO_3)_3 \cdot 9H_2O$	0.10	—
Valine	94.00	20.00	$NaH_2PO_4 \cdot H2O$	141.30	—
Isoleucine	104.80	50.00	Vitamin B12	—	0.005
Leucine	104.80	50.00	$Ca(NO_3)_2 \cdot 4H_2O$	—	100.00
Lysine	146.00	40.00	Na_2HPO_4	—	800.70
Methionine	30.00	15.00	Hydroxyproline	—	20.00
Phenylalanine	66.00	15.00	HEPES	—	5958.00
Serine	42.00	30.00	Biotin	—	0.20
Threonine	95.00	20.00	Proline	—	20.00
Tryptophane	16.00	5.00	Asparagine	—	50.00
Tyrosine	72.00	23.19	Asparate	—	20.00
NaCl	6400.00	6000.00	Cysteine	—	50.00
KCl	400.00	400.00	Glutamate	—	20.00
Calciate	4.00	0.25	Pyridoxine	—	1.00

Table S2 Resonance assignments of metabolites in ^{1}H NMR spectra of aqueous extracts from SGC7901 cells originally cultured in RPMI1640 and DMEM.

Metabolites and Abbreviation	δ ^{1}H (ppm) and multiplicity	Moieties
Isoleucine(Ile)	0.94(t); 1.01(d); 1.21(m); 1.42(m); 2.00(m); 3.67(d)	δ-CH_3 ; γ-CH_3; half γ-CH_2; half γ-CH_2; β-CH; α-CH
Leucine(Leu)	0.96(d); 0.97(d); 1.69(m); 1.70(m); 1.73(m); 3.73(m)	α-CH_3; α-CH_3; γ-CH; β-CH_2; α-CH
Valine(Val)	0.99(d); 1.05(d); 2.26(m); 3.60(d)	γ-CH_3; γ-CH_3; β-CH; α-CH
Lactate(Lac)	1.33(d);4.11(q)	β-CH_3; α-CH
Threonine(Thr)	1.30(d); 3.58(d); 4.24(m)	γ-CH_2; β-CH
Alanine(Ala)	1.47(d); 3.78(q)	β-CH_3; α-CH
N-Acetylgly-coproteins(NAC)	2.04(s)	CH_3
Pyroglutamate(PG)	2.05(m); 2.39(d); 2.51(m); 4.18(dd)	β-CH; γ-CH_2; β-CH; α-CH
Aspartate(Asp）	2.68(dd); 2.81(dd); 3.90(dd)	β-CH_2; α-CH
Choline(Cho)	3.21(s); 3.51(dd); 4.04(t)	N-$(CH_3)_3$; N-CH_2; CH_2OH
Phosphocholine(PC)	3.22(s); 3.60(t); 4.18(m)	N-$(CH_3)_3$; N-CH_2; CH_2OH
Glycero-3-phosphocholine(GPC)	3.23(s); 3.60(dd); 3.68(dd); 3.87(m); 3.94(m); 4.33(m)	N-$(CH_3)_3$; half $^{1}CH_2$; $^{2}CH_2$; half $^{1}CH_2$; half $^{3}CH_2$; half $^{3}CH_2$; $^{1}CH_2$
Taurine(Tau)	3.27(t); 3.43(t)	$^{1}CH_2$; $^{2}CH_2$
Glycine(Gly)	3.57(s)	α-CH_2
Glutamate(Glu)	2.08(m); 2.12(m); 2.34(m); 2.37(m); 3.75(m)	half β-CH_2; half β-CH_2; half γ-CH_2; half γ-CH_2; α-CH
Glutamine(Gln)	2.13(m); 2.45(m); 3.77(t)	γ-CH_2; β-CH_2; α-CH
Creatine Phosphoate(PCr)	3.05(s); 4.05(s)	N-CH_3; CH_2
Creatine(Cr)	3.04(s); 3.93(s)	N-CH_3; α-CH_2
Proline(Pro)	1.99(m)	γ-CH_2
Tyrosine(Tyr)	3.05(dd); 3.19(dd); 6.92(d); 7.19(d)	half β-CH_2; half β- CH_2;β-CH; α-CH
Phenylalanine(Phe)	3.12(dd); 3.30(dd); 3.99(dd); 7.33(d); 7.37(t); 7.43(t)	α-CH; half-β-CH_2; half β-CH_2; α-CH; β-CH; γ-CH
Formate(For)	8.46(s)	CH
Nicotinamide adenine dinuclectide(NAD)	6.03(d); 6.08(s); 8.16(s); 8.20(m); 8.41(s); 8.82(d); 9.13(d); 9.32(s)	NH_2; NH_2(CO); δ-CH; β-CH; 2CH; γ-CH; α-CH;
Adenosine Triphosphate(ATP)	6.14(d); 8.27(s); 8.58(s)	NH_2; δ-CH; 2CH

Table S3 K-means clustering analysis of ^{1}H NMR data of aqueous extracts from SGC7901 cells during the gradual acclimation from RPMI1640 to DMEM.

	Samples in each cluster
Cluster(1)	R-D 1-1；R-D 1-2；R-D 1-3；R-D 1-4；R-D 1-5；R-D 1-6； R-D 2-1；R-D 2-2；R-D 2-3；R-D 2-4；R-D 2-5；R-D 2-6； R-D 4-1；R-D 4-2；R-D 4-3；R-D 4-4；R-D 4-5；R-D 4-6.
Cluster(2)	D-1；D-2；D-3；D-4；D-5；D-6； R-D 6-1；R-D 6-2；R-D 6-3；R-D 6-4；R-D 6-5；R-D 6-6； R-D 8-1；R-D 8-2；R-D 8-3；R-D 8-4；R-D 8-5；R-D 8-6.
Cluster(3)	R-1；R-2；R-3；R-4；R-5；R-6.

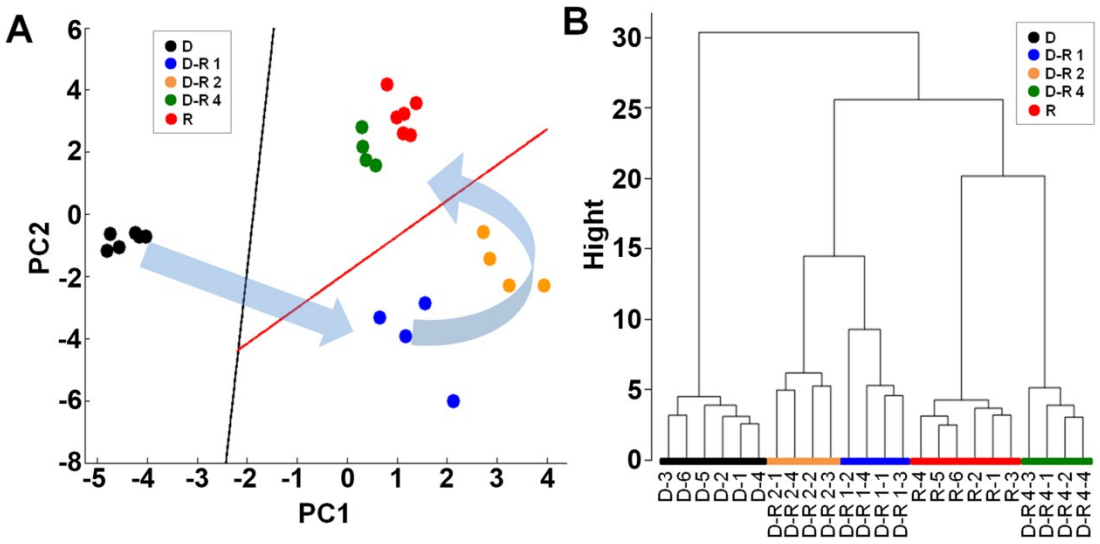

Fig. S2 (A) PCA scatter plot and (B) hierarchical cluster analysis result of ^{1}H NMR data of aqueous extracts from SGC7901 during the acclimation from DMEM to RPMI1640, which illustrates the changes of metabolic profiles after 1, 2, 4 times of subculture.

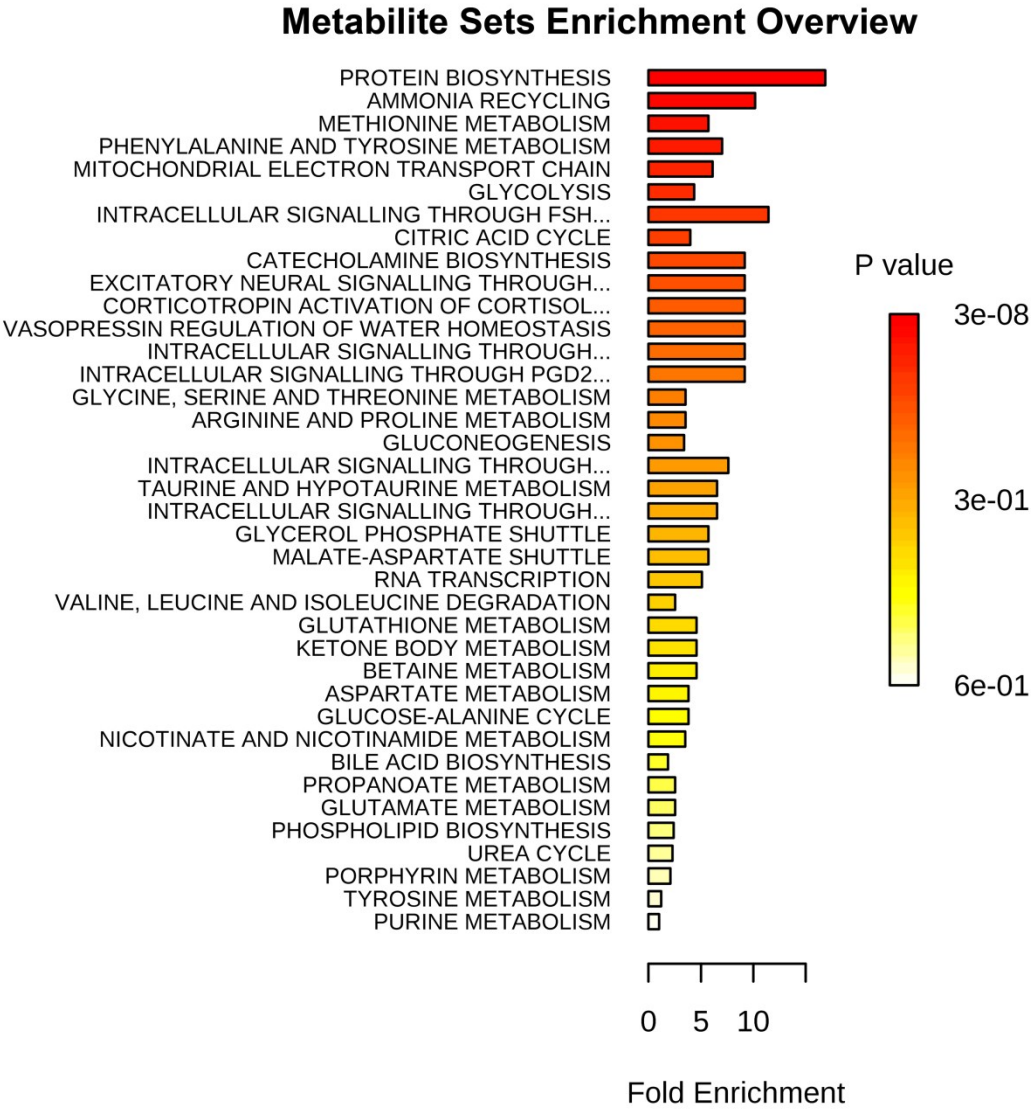

Fig. S3 Metabolite set enrichment analysis (MESA) result of discrepant metabolites.