Supporting information for

Mass spectrometry-based lipidomics analysis using methyl tertbutyl ether extraction in human hepatocellular carcinoma tissues

Shuxia Jiang^{a,b}, Yongle Li^c, Shuhai Lin^b, HongboYang^c, Xin-yuan Guan^d, Haiyun Zhou^{a,*}, Tiangang Luan^{a,e}, Zongwei Cai^{b,*}

^a Instrumental Analysis & Research Center, Sun Yat-sen University, Guangzhou, 510275, China. E-mail: zhouhy@mail.sysu.edu.cn.

^b State Key Laboratory of Environmental and Biological Analysis and Department of Chemistry, Hong Kong Baptist University, Kowloon,

Hong Kong SAR, China. Fax: +852-3411 7348; Tel: +852-3411 7070; E-mail: zwcai@hkbu.edu.hk

^c Shenzhen Academy of Metrology and Quality Inspection, Shenzhen, 518000, China

^d Department of Clinical Oncology, Li KaShing Faculty of Medicine, the University of Hong Kong, Hong Kong SAR, China

^e MOE Key Laboratory of Aquatic Product Safety, School of Life Sciences, Sun Yat-sen University, Guangzhou, 510275, China



Figure S1. Full scan base peak mass chromatograms in positive mode: (A) ANT group, (B) HCTgroup.



Figure S2. TG were synthesized form glycerol-3-phosphate initially, and catalyzed by sn-1glycerol-3-phosphate acyltransferase to form lysophosphatidic acid (LPA). Then LPA form phosphatidic acid (PA) under the function of acylCoA: 1-acylglycerol-3-phosphate acyltransferase. DG is formed from PA by hydrolyzed by PA phosphatase. Finally, DG is esterified by DG acyltransferase to synthesize TG.



Figure S3. Abbreviations: Cho K, choline kinase; Eth K,ethanolamine kinase; CCT, phosphocholine (or phosphethanolamine) cytidylyltransferase;CPT, cholinephosphotransferase; EPT,ethanolaminephosphotransferase;PEMT, phosphatidylethanolamine N-methyltransferase; CDS, CDP-diacylglycerol synthase; PGS, phosphatidylglycerol synthase; PSS,phosphatidylserine synthase; PSD, phosphatidylserine decarboxylase; PIS, phosphatidylinositol synthase;
P-Cho, phosphocholine; P-Eth, phosphoethanolamine; CDP-Cho, CDP-choline; CDP-Eth, CDP-ethanolamine; PA, phosphatidic acid; PC, phosphatidylcholine; PE, phosphatidylethanolamine; PG, phosphatidylglycerol; PS, phosphatidylserine; PI,

phosphatidylinositol.