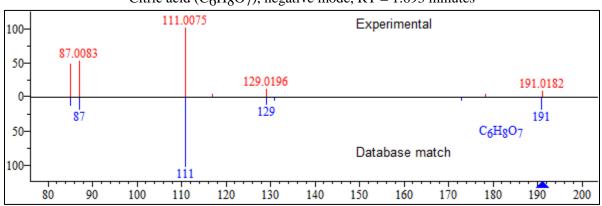
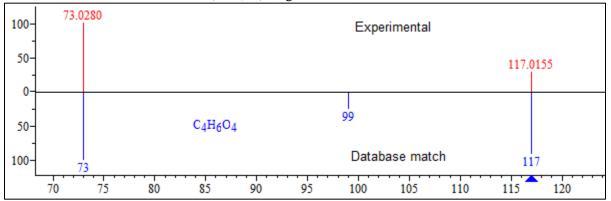
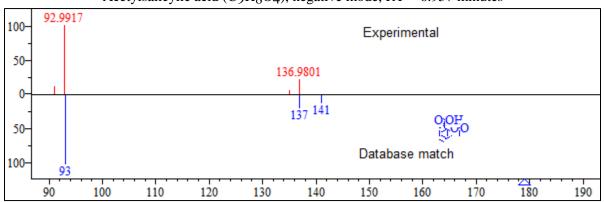
Additional file 5: Tandem MS fragmentation patterns for six EBC metabolites. The mass spectral fragment peaks in red indicate the experimental results. The peaks in blue indicate the database matches based on standards.



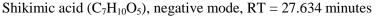
Citric acid ($C_6H_8O_7$), negative mode, RT = 1.693 minutes

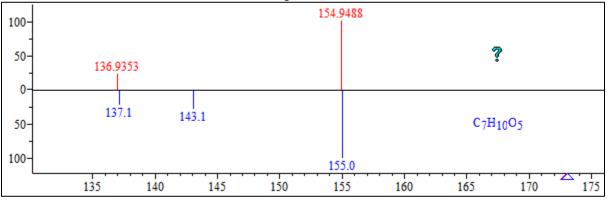


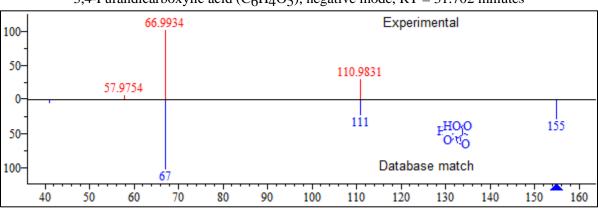
Succinic acid ($C_4H_6O_4$), negative mode, RT = 1.830 minutes



Acetylsalicylic acid (C9H8O4), negative mode, RT = 6.957 minutes







3,4-Furandicarboxylic acid (C₆H₄O₅), negative mode, RT = 31.702 minutes

4-Chloro-L-phenylalanine (C9H₁₀ClNO₂), negative mode, RT = 31.518 minutes

