

 $201622\_pHILIC\_\_POS\_MSMS\_KBL\_Qex\_Root\_BrachyExudate\_22\_time\_1\_hr\_\_Run54.h5$ 

betaalanine\_betaine\_positive\_5p97

m/z theoretical = 132.1019, measured = 132.1017, 1.0529 ppm difference

Expected Elution of 5.97 minutes, 6.18 min actual

