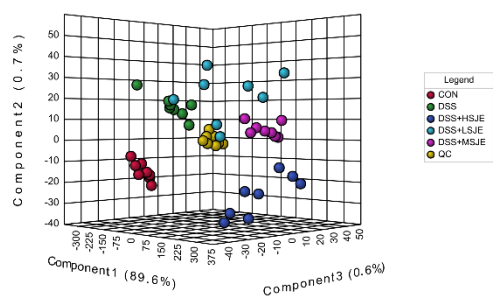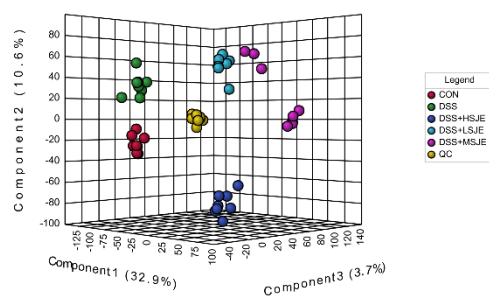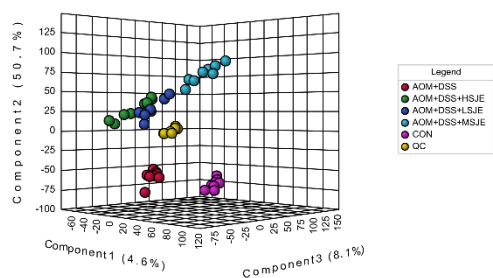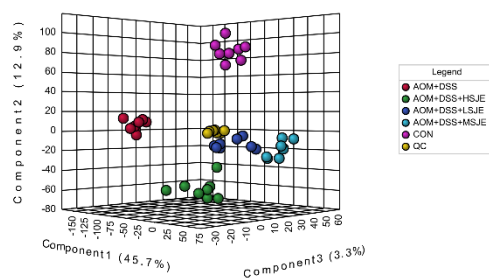Figure S1. PLS-DA analysis of all samples. PLS-DA plots of all samples from UC experiments in negative ion mode (A) and positive ion mode (B). PLS-DA plots of all samples from CAC experiments in negative ion mode (C) and positive ion mode (D).