

Table S2

Measured S881 Fragment Mass	Assigned Elemental Composition	Theoretical Exact Mass
79.95	SO ₃	79.95
96.96	HSO ₄ ⁻	96.96
163.00	C ₅ H ₇ O ₄ S ₁ ⁻	163.00
172.05	C ₁₁ H ₈ O ₂ ⁻	172.05
185.06	C ₁₂ H ₉ O ₂ ⁻	185.06
231.07	C ₁₀ H ₁₅ O ₄ S ₁ ⁻	231.07
299.13	C ₁₅ H ₂₃ O ₄ S ₁ ⁻	299.13
367.20	C ₂₀ H ₃₁ O ₄ S ₁ ⁻	367.19
695.50	C ₄₄ H ₇₁ O ₄ S ₁ ⁻	695.51
783.56	C ₅₆ H ₇₉ O ₂ ⁻	783.61
786.57	C ₅₅ H ₇₈ O ₃ ⁻	786.59
801.59	C ₅₆ H ₈₁ O ₃ ⁻	801.62
881.61	C ₅₆ H ₈₁ O ₆ S ₁ ⁻	881.58