

Supplementary Materials

Supplementary Data S5. LC-ESIMS Data for Detecting 1-3 in EtOAc Extracts of G59 and Its Mutant BD-1-6

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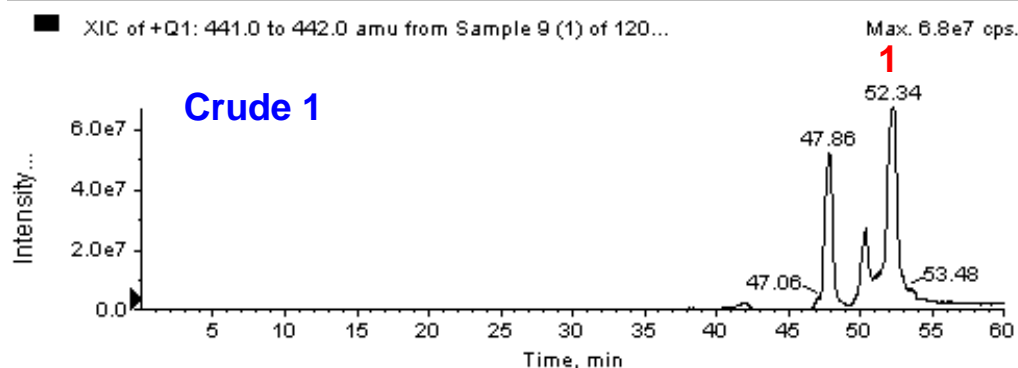
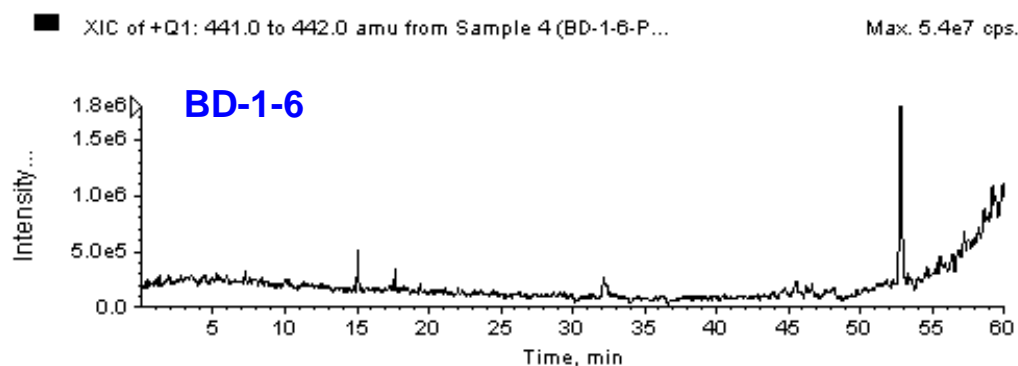
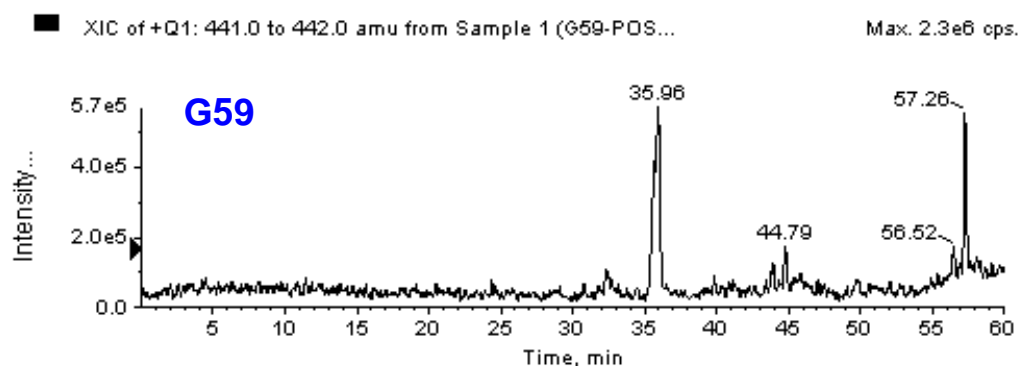
1. Conditions and conclusions of LC-ESIMS analysis to detect compounds **1-3**

Conditions: LC-ESIMS analysis was performed on a LC-MS equipment equipped with Agilent 1100 HPLC system, AB Sciex API 3000 LC-MS/MS system, and AB Sciex Analyst 1.4 software. EtOAc extracts of G59 and BD-1-6 were employed for the LC-ESIMS analysis and crude **1–3** samples were used as control. HPLC was carried out on a Venusil MP C18 column (5 μ m, 100 Å, 4.6 mm \times 250 mm; Agela Technologies) using MeOH–H₂O in linear gradient (20% MeOH at initial time 0 min \rightarrow 100% MeOH at 60 min \rightarrow 100% MeOH at 90 min; flow rate, 1 ml/min) as mobile phase. The mass detector was set to scan a range from m/z 150 to 1500 in positive (for **1–3**) or negative (for **1**) mode. The acquired data were processed by Analyst 1.4 software to obtain targeted LC-ESIMS data.

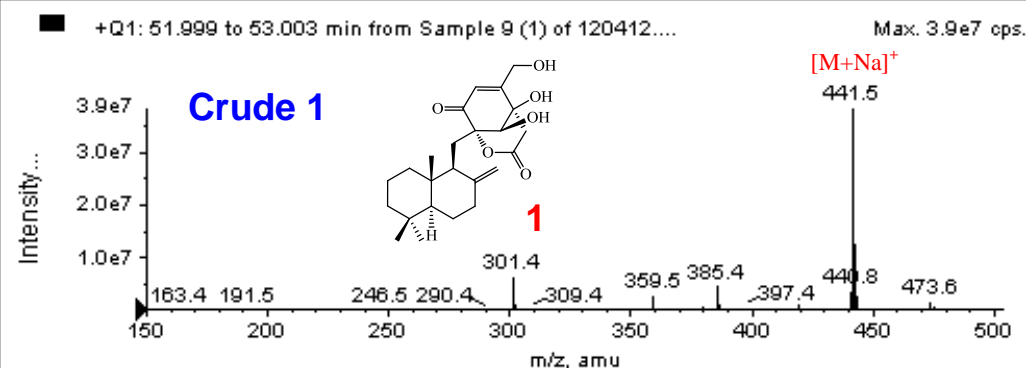
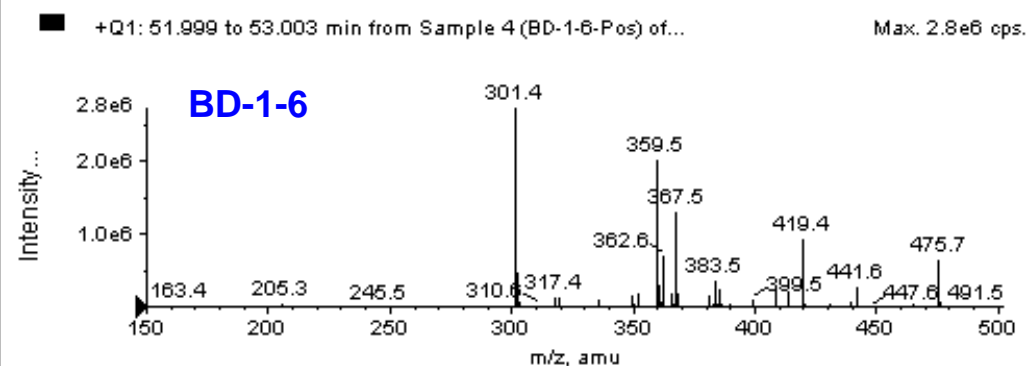
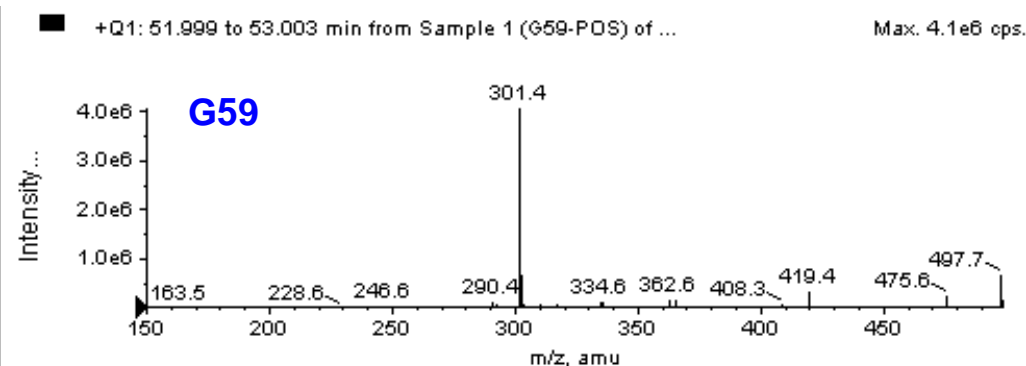
Conclusions: The $[M+Na]^+$ or $[M-H]^-$ ions of **1**, **2**, and **3** were appeared as peaks with retention times of 52.3, 53.8, and 55.1 min, respectively. Compounds **1–3** in BD-1-6 and G59 were examined by using selective ion monitoring and all of **1–3** were detected only in BD-1-6 but entirely not in G59 samples.

LC-ESIMS Data for Detecting 1 ($[M+Na]^+$ ion) in Parent G59 and Its Mutant BD-1-6 Samples

Positive Selective Ion (m/z 441.0-442.0) Monitoring Chromatograms

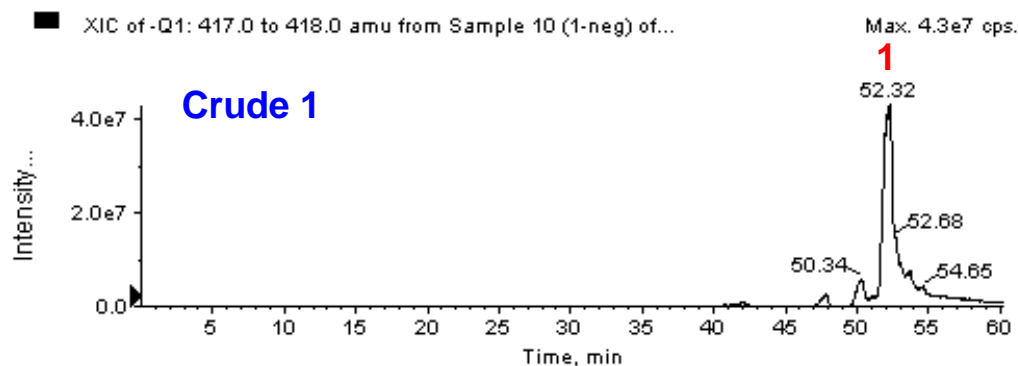
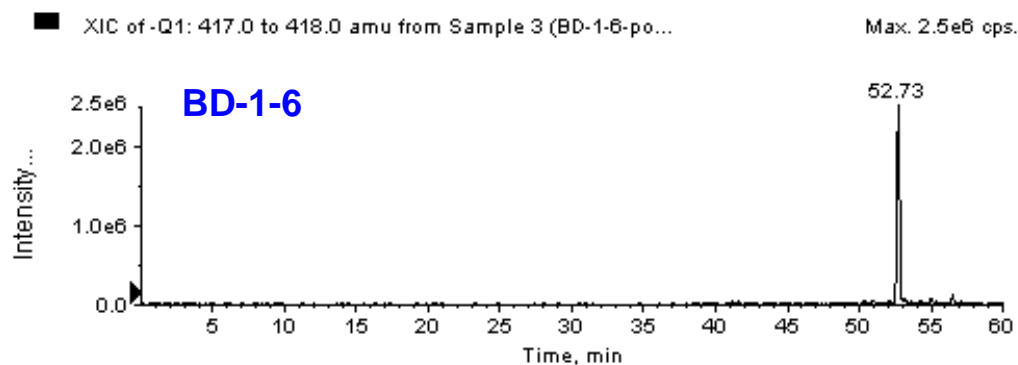
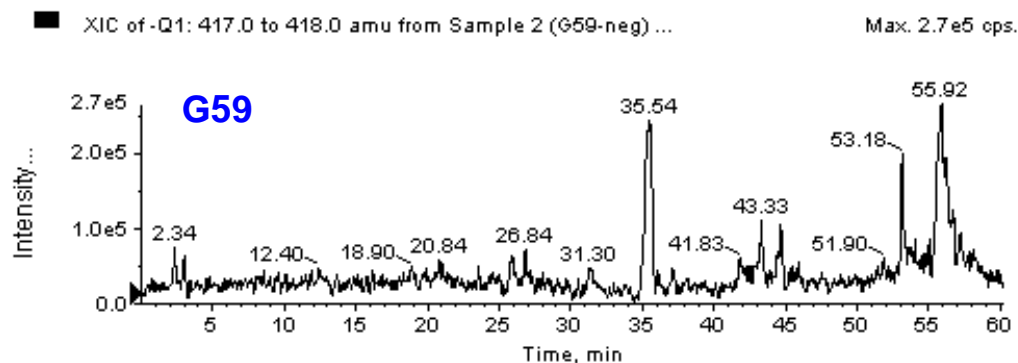


ESIMS Spectra in the Range of 51.999-53.003 min Retention Times

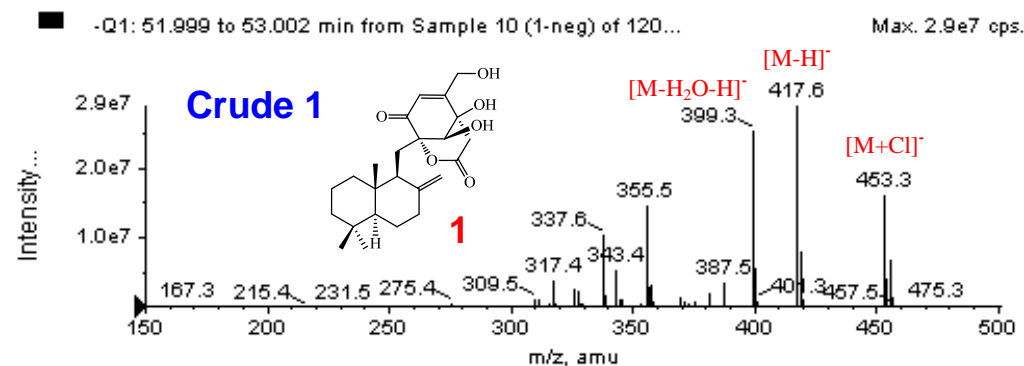
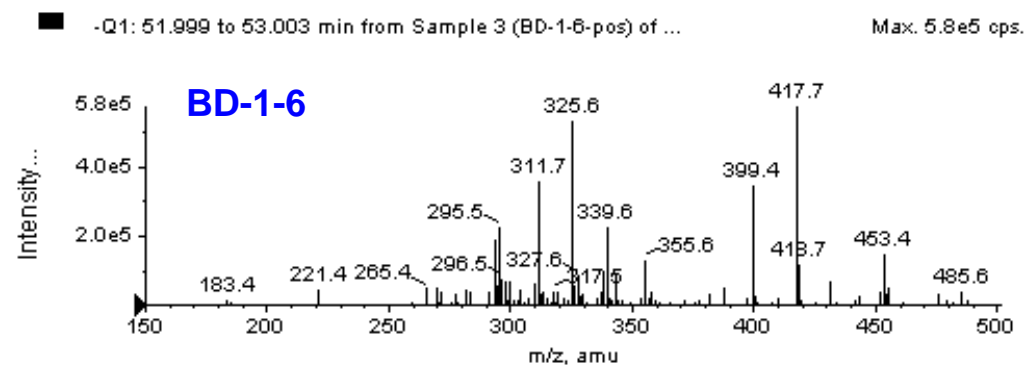
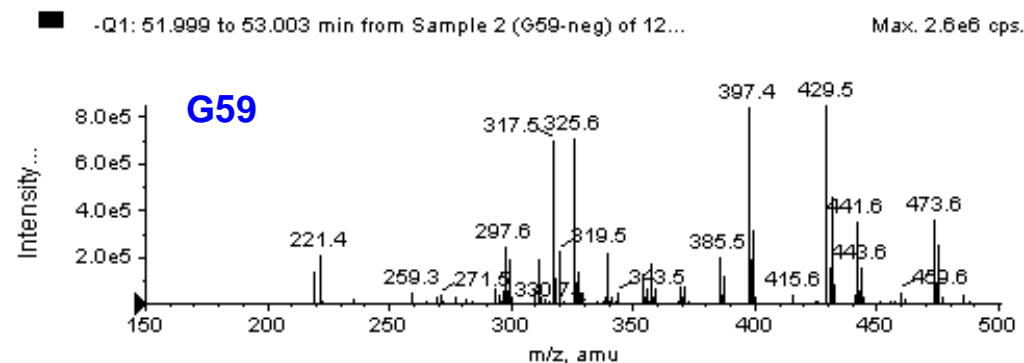


LC-ESIMS Data for Detecting 1 ($[M-H]^-$ ion) in Parent G59 and Its Mutant BD-1-6 Samples

Negative Selective Ion (m/z 417.0-418.0) Monitoring Chromatograms

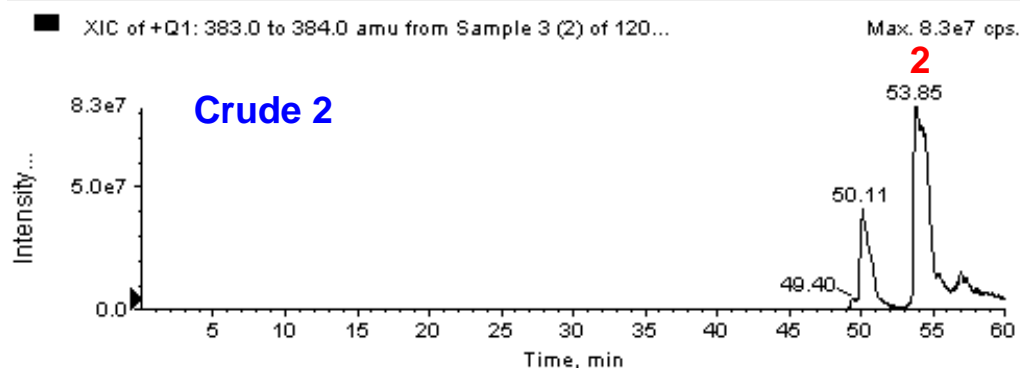
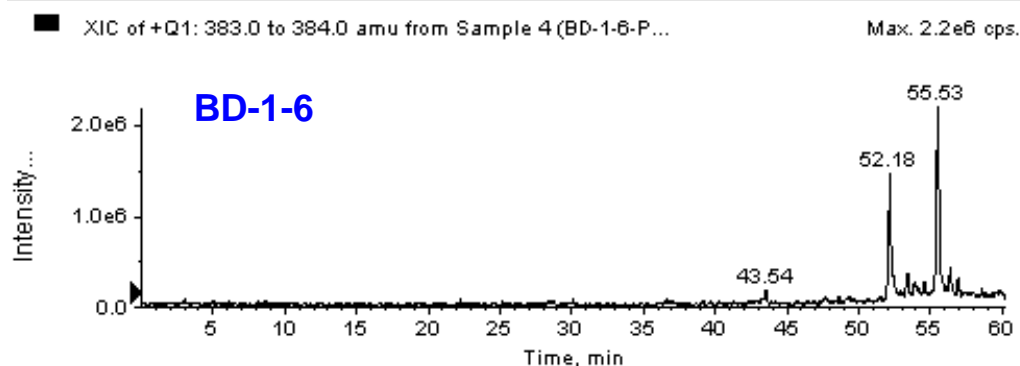
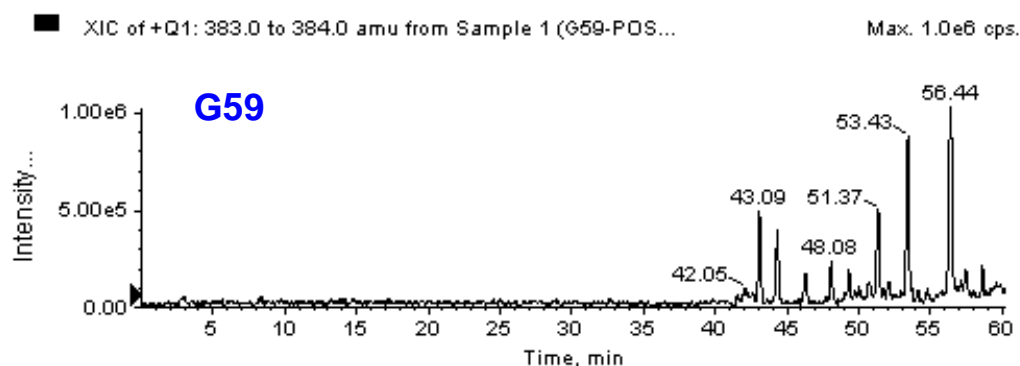


ESIMS Spectra in the Range of 51.999-53.003 min Retention Times

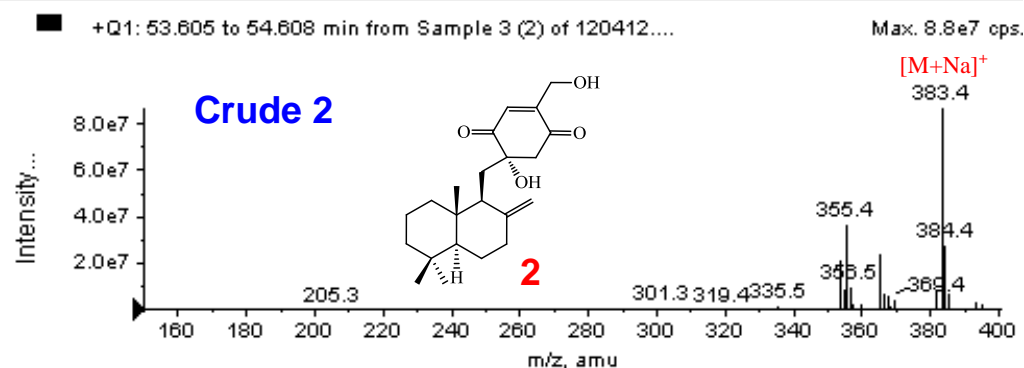
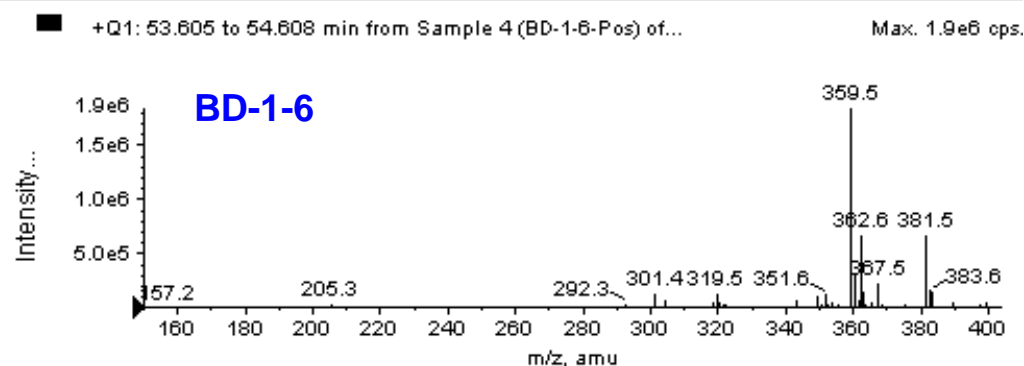
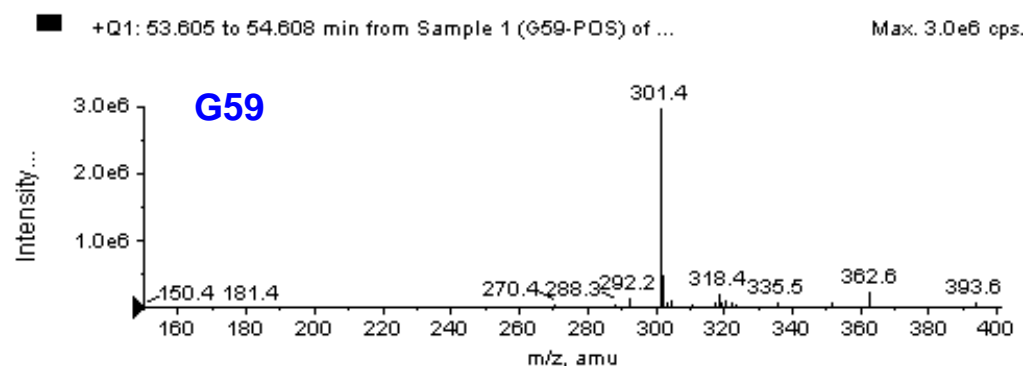


LC-ESIMS Data for Detecting 2 ($[M+Na]^+$ ion) in Parent G59 and Its Mutant BD-1-6 Samples

Positive Selective Ion (m/z 383.0-384.0) Monitoring Chromatograms

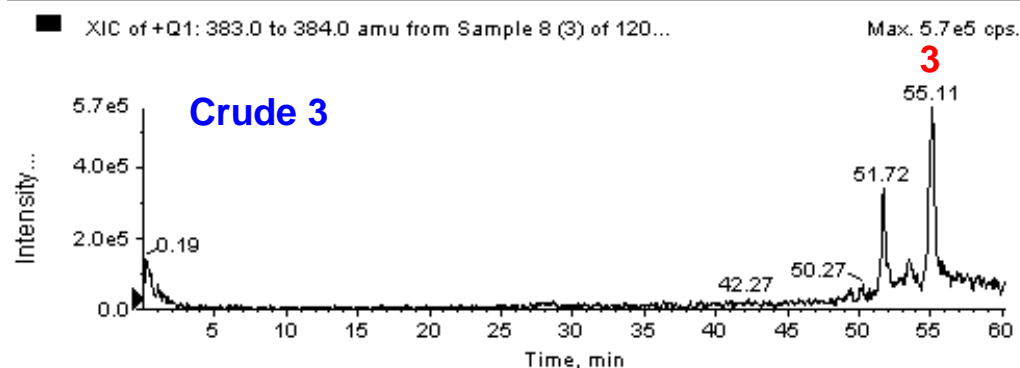
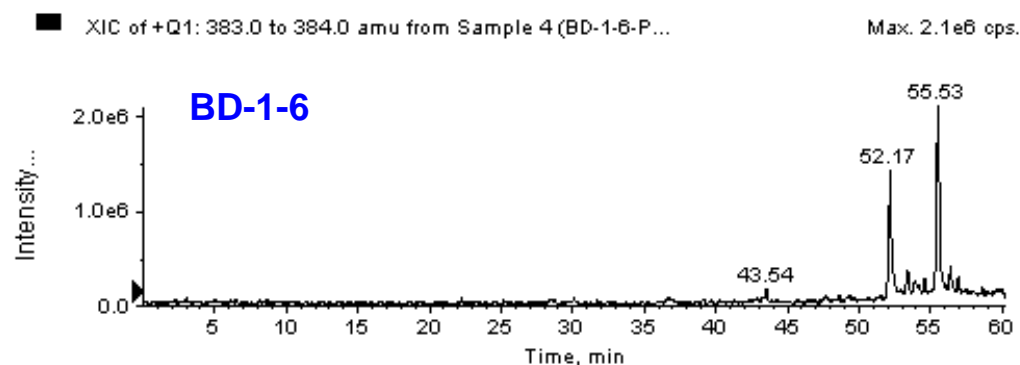
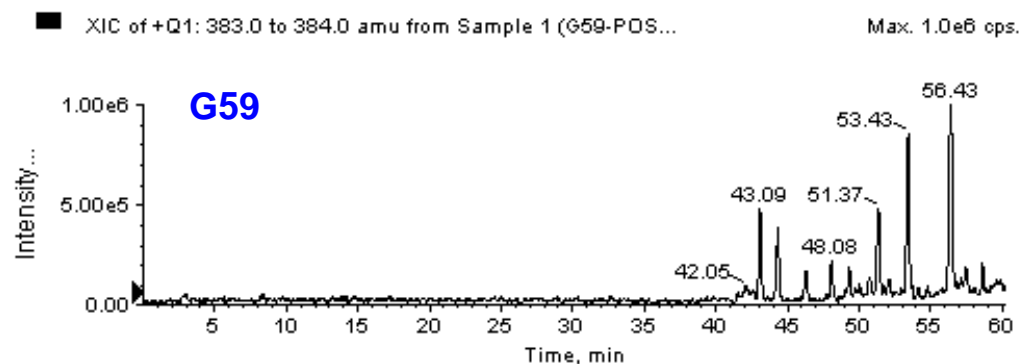


ESIMS Spectra in the Range of 53.605-54.608 min Retention Times



LC-ESIMS Data for Detecting **3** ($[M+Na]^+$ ion) in Parent G59 and Its Mutant BD-1-6 Samples

Positive Selective Ion (m/z 383.0-384.0) Monitoring Chromatograms



ESIMS Spectra in the Range of 54.708-55.511 min Retention Times

