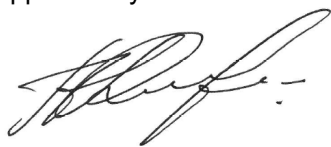


<b>Name:</b>	<b>1β-Hydroxydeoxycholeic Acid-D4 (major)</b>
<b>Lot#:</b>	GR-7-031
<b>Test Date:</b>	02/10/2025 (re-test date: 02/10/2030)
<b>CAS No.:</b>	80434-32-8 (unlabeled)
<b>MF:</b>	C <sub>24</sub> H <sub>36</sub> D <sub>4</sub> O <sub>5</sub>
<b>MW:</b>	412.53
<b>Appearance:</b>	White solid
<b>Purity:</b>	~97% by NMR; ~98% atom D; TLC – one spot (eluent – EtOAc)
<b><sup>1</sup>H-NMR:</b>	Conforms
<b>MS-ESI (-)</b>	Conforms (shows peak at m/z = 411.31 [M-H] <sup>-</sup> )
<b>Storage</b>	Store at -18°C in a dry place away from direct sunlight

Approved by:

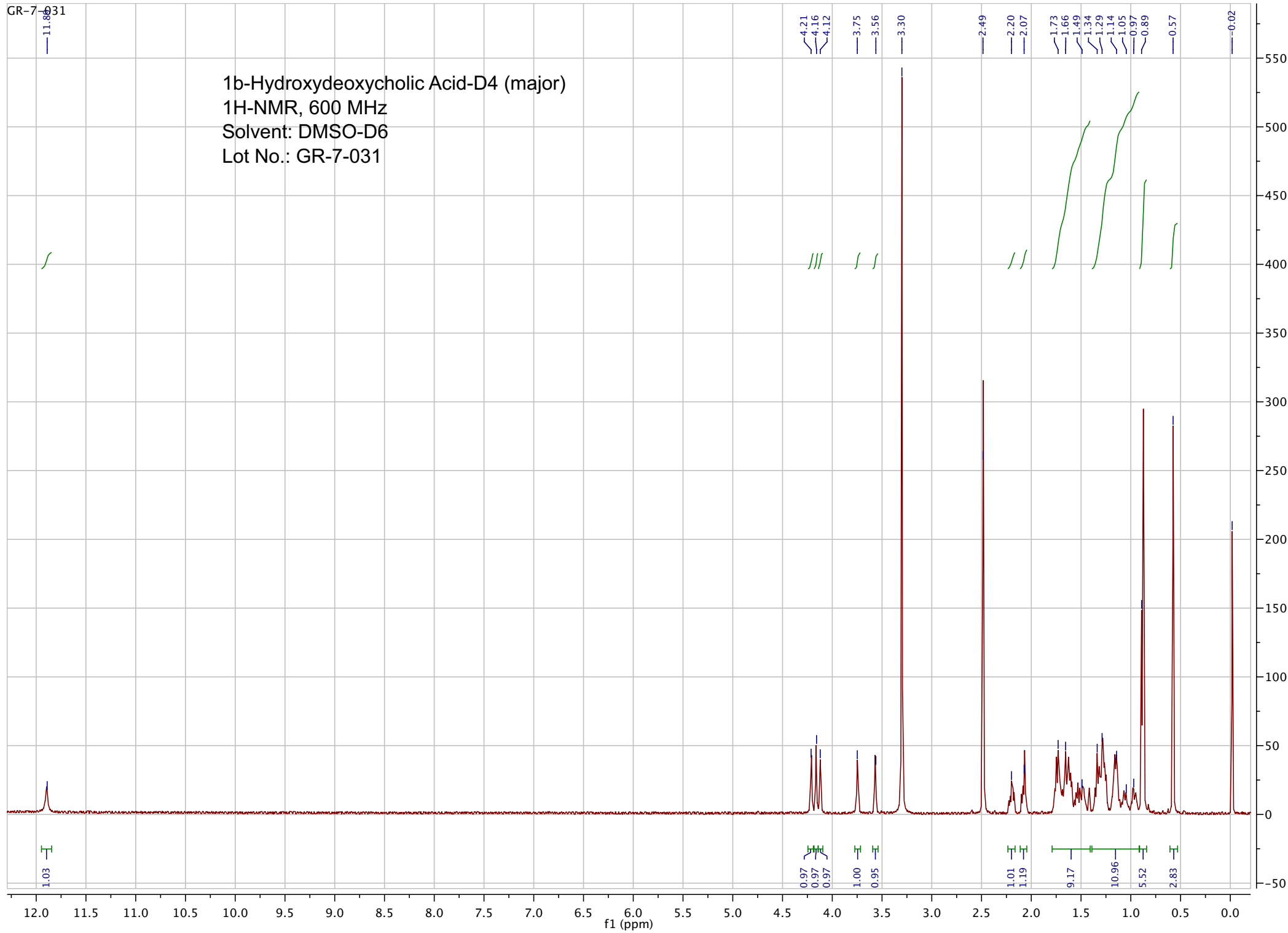
Date: 02/10/2025



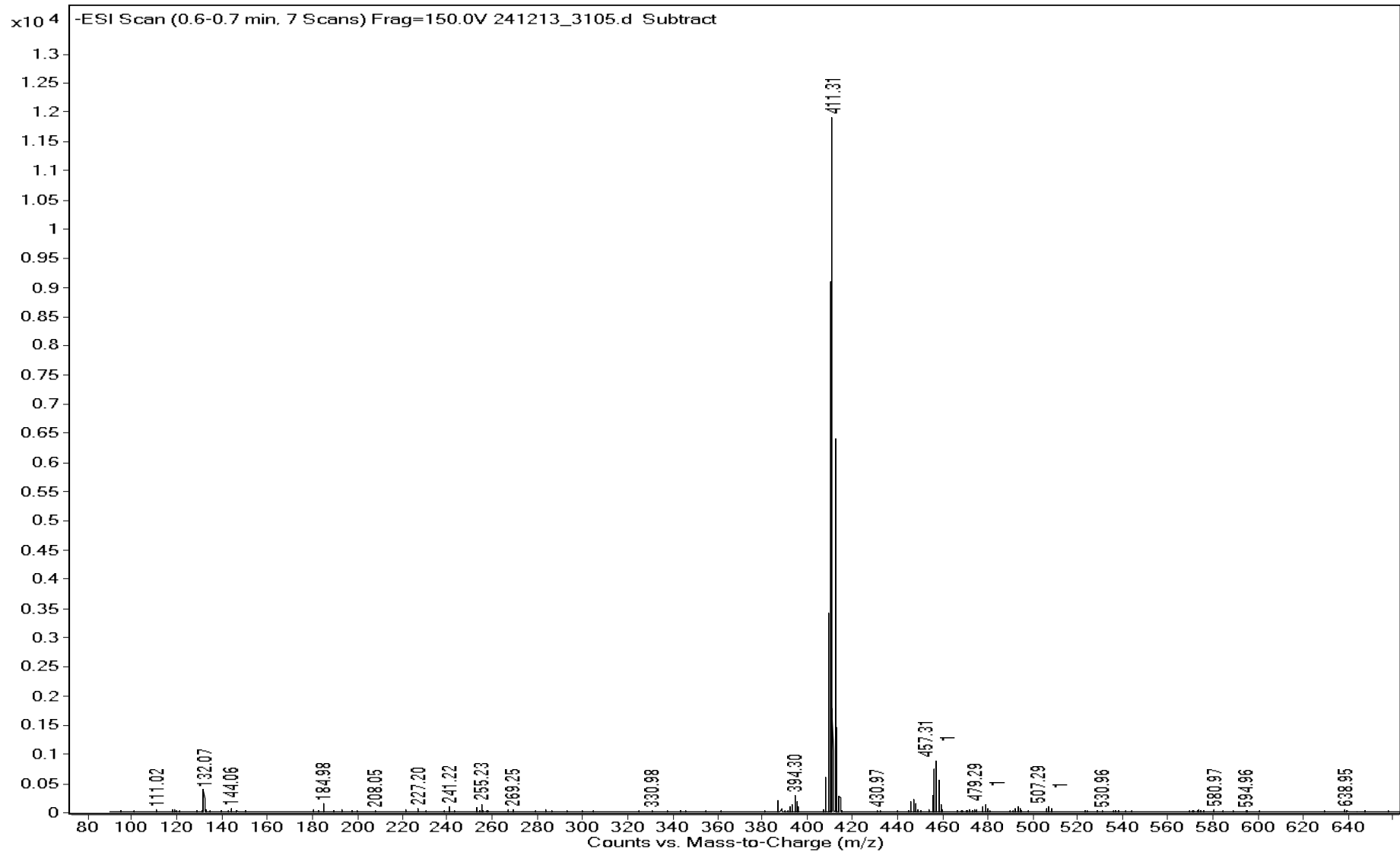
Viorica Rusu, QC/QA Manager

GR-7-031

1b-Hydroxydeoxycholic Acid-D4 (major)  
1H-NMR, 600 MHz  
Solvent: DMSO-D6  
Lot No.: GR-7-031



<b>Sample Name</b>	GR-7-031	<b>Data File</b>	241213_3105.d	<b>Acq Method</b>	HRMS_Negative.m
<b>DA Method</b>	AIMS_Accurate_Mass.m	<b>Instrument</b>	Agilent 6538 UHD	<b>Acq Date, Time</b>	13/12/2024 4:10:41 PM
<b>Comment</b>	ESI-				



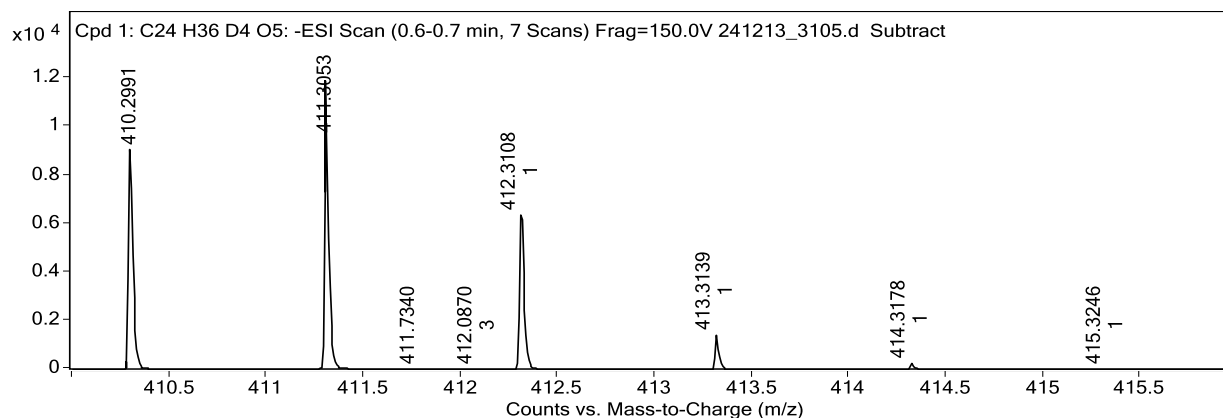
<b>Sample Name</b>	GR-7-031	<b>Data File</b>	241213_3105.d
<b>Acq Method</b>	HRMS_Negative.m	<b>DA Method</b>	AIMS_Accurate_Mass.m
<b>Instrument</b>	Agilent 6538 UHD	<b>Acq Date, Time</b>	13/12/2024 4:10:41 PM
<b>Comment</b>	ESI-		

### Target Ion Species

Ion Species	m/z	Ionic Formula
(M-H) <sup>-</sup>	411.3053	C24 H35 D4 O5

### MFG Calculator Results

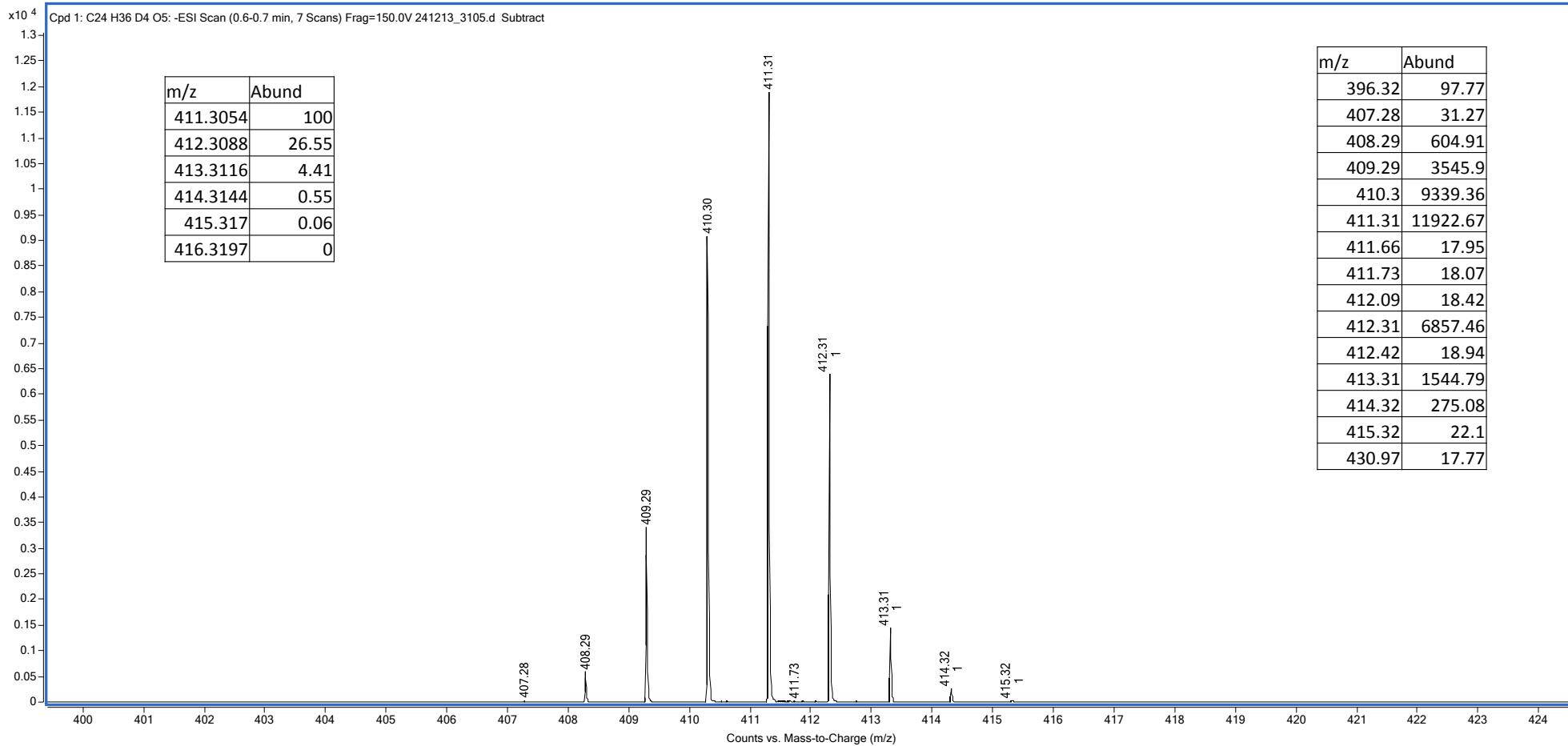
Target m/z	Ionic Formula	Calc m/z	+/- (mDa)	+/- (ppm)	DBE	MFG Score
411.3053	C24 H35 D4 O5	411.3054	-0.1	-0.2	5.0	62.48
411.3053	C25 H31 D4 N4 O	411.3067	-1.4	-3.4	10.0	56.05



### Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	411.3053	411.3054	-0.1	100.0	100.0	0.0

Cpd 1: C24 H36 D4 O5: -ESI Scan (0.6-0.7 min, 7 Scans) Frag=150.0V 241213\_3105.d Subtract



m/z	Abund
411.3054	100
412.3088	26.55
413.3116	4.41
414.3144	0.55
415.317	0.06
416.3197	0

m/z	Abund
396.32	97.77
407.28	31.27
408.29	604.91
409.29	3545.9
410.3	9339.36
411.31	11922.67
411.66	17.95
411.73	18.07
412.09	18.42
412.31	6857.46
412.42	18.94
413.31	1544.79
414.32	275.08
415.32	22.1
430.97	17.77