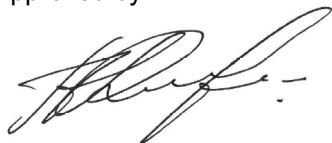


Name:	1β-Hydroxydeoxycholic Acid Acyl Glucuronide
Lot#:	GR-19-209
Test Date:	12/20/2024 (re-test date: 12/20/2027)
CAS No.:	NA
MF:	C ₃₀ H ₄₈ O ₁₁
MW:	584.70
Appearance:	Off-White solid
Purity:	>95% by NMR; TLC(C18) – one spot (eluent 40% EtOAc in Acetone)
¹H-NMR:	Conforms (shows a trace of EtOAc and ~1% Tetramethylurea)
MS-ESI (-)	Conforms (shows peak at m/z = 583.31 [M-H] ⁻)
Storage	Store at -18°C in a dry place away from direct sunlight

Approved by:

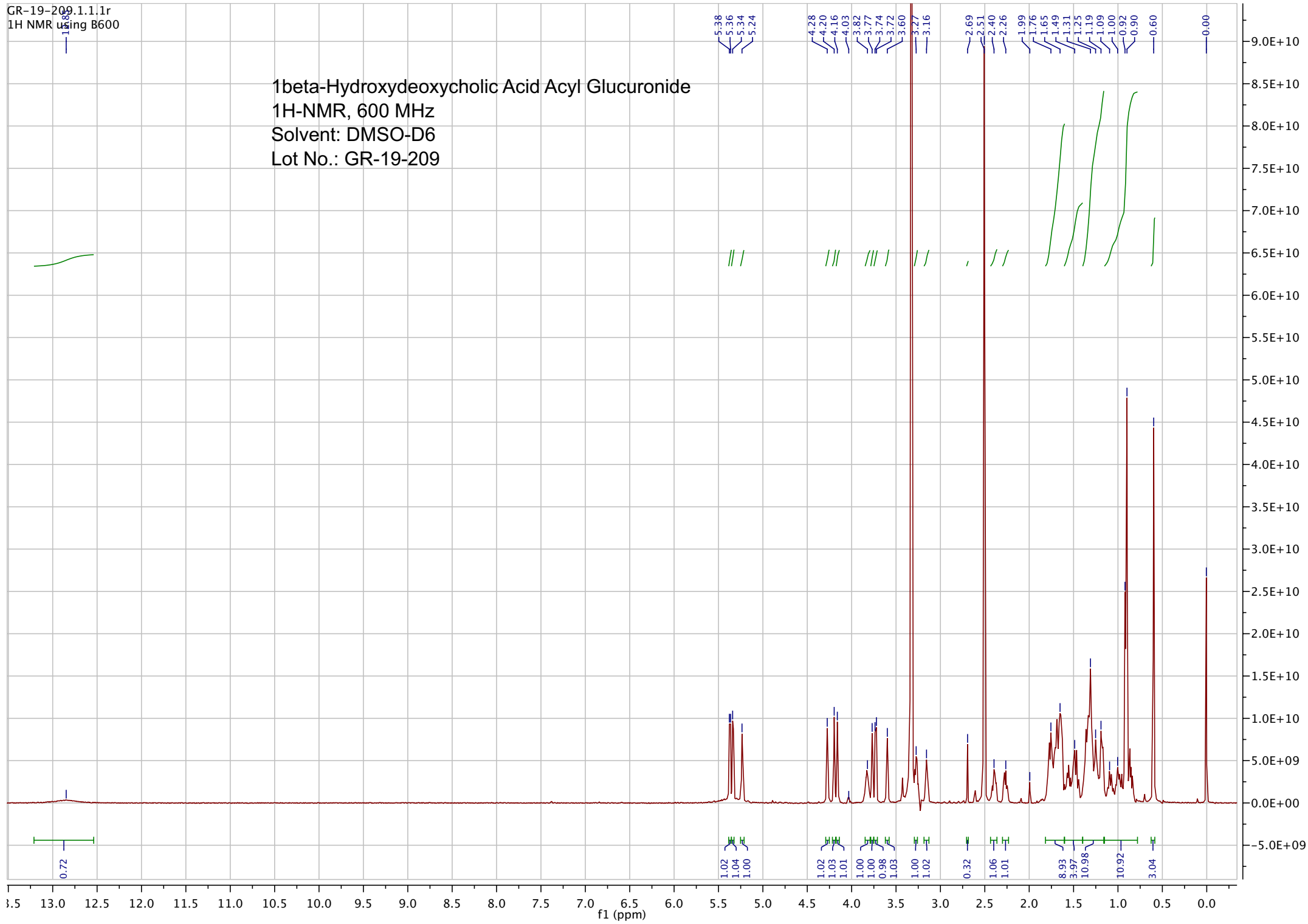
Date: 12/21/2024



Viorica Rusu, QC/QA Manager

GR-19-209.1.1.1r
1H NMR using B600

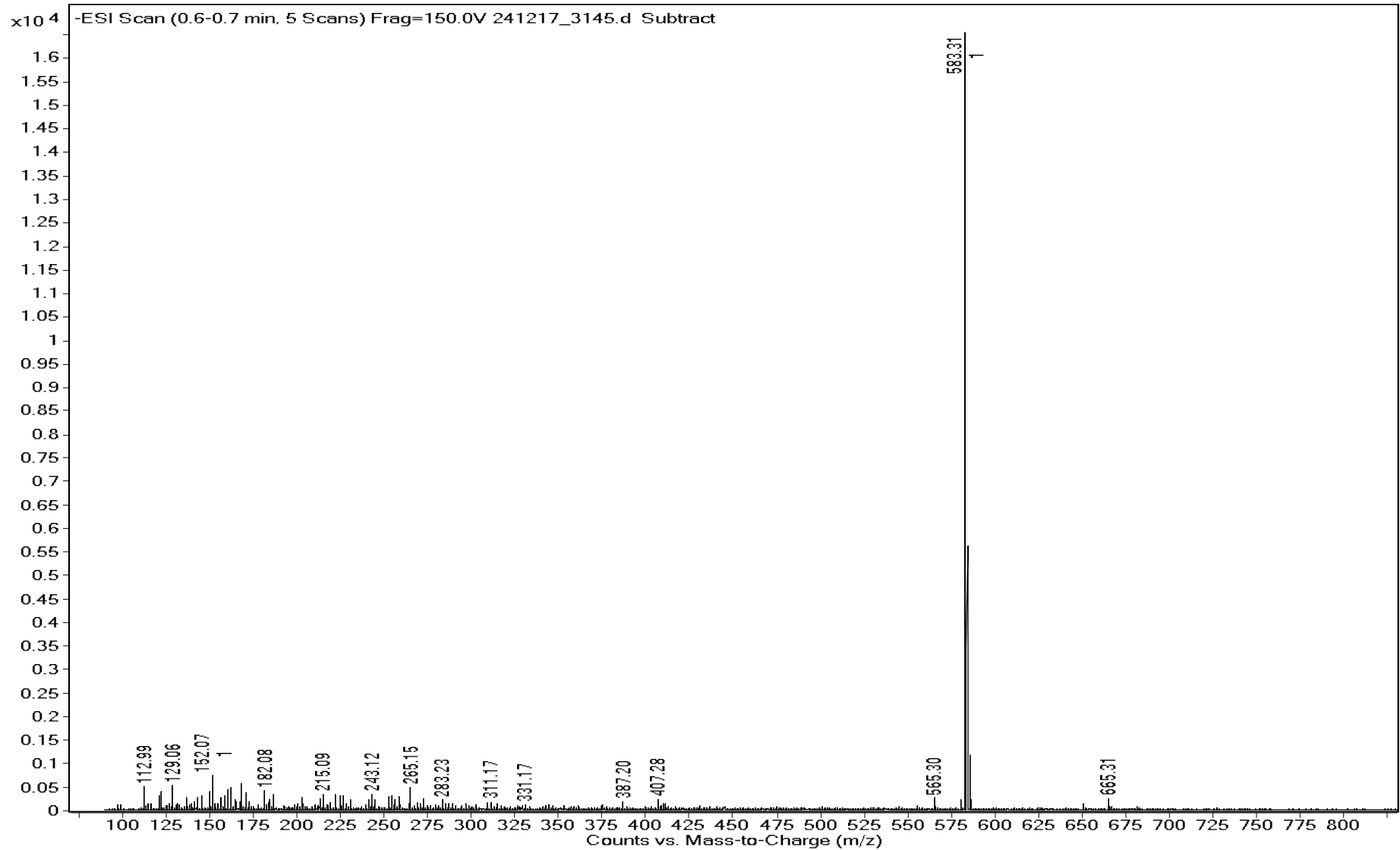
1beta-Hydroxydeoxycholic Acid Acyl Glucuronide
1H-NMR, 600 MHz
Solvent: DMSO-D6
Lot No.: GR-19-209



Sample Name GR-19-209
DA Method AIMS_Accurate_Mass.m
Comment ESI-

Data File 241217_3145.d
Instrument Agilent 6538 UHD

Acq Method HRMS_Negative.m
Acq Date, Time 17/12/2024 4:09:25 PM



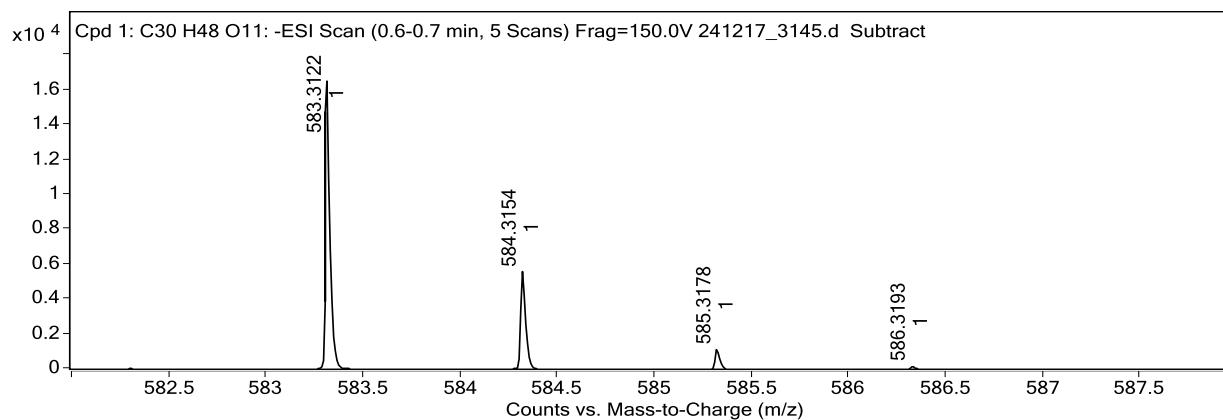
Sample Name	GR-19-209	Data File	241217_3145.d
Acq Method	HRMS_Negative.m	DA Method	AIMS_Accurate_Mass.m
Instrument	Agilent 6538 UHD	Acq Date, Time	17/12/2024 4:09:25 PM
Comment	ESI-		

Target Ion Species

Ion Species	m/z	Ionic Formula
(M-H) ⁻	583.3122	C30 H47 O11

MFG Calculator Results

Target m/z	Ionic Formula	Calc m/z	+/- (mDa)	+/- (ppm)	DBE	MFG Score
583.3122	C30 H47 O11	583.3124	-0.2	-0.3	7.0	99.23
583.3122	C27 H39 N10 O5	583.3110	1.2	2.1	13.0	96.67
583.3122	C31 H43 N4 O7	583.3137	-1.5	-2.6	12.0	95.43
583.3122	C26 H43 N6 O9	583.3097	2.5	4.3	8.0	88.55
583.3122	C32 H39 N8 O3	583.3151	-2.9	-5.0	17.0	85.95
583.3122	C43 H39 N2	583.3119	0.3	0.5	25.0	85.72
583.3122	C25 H47 N2 O13	583.3084	3.8	6.5	3.0	76.44
583.3122	C38 H39 N4 O2	583.3079	4.3	7.4	21.0	68.67
583.3122	C20 H43 N10 O10	583.3169	-4.7	-8.1	4.0	66.69



Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	583.3122	583.3124	-0.2	100.0	100.0	0.0
2	584.3154	584.3158	-0.4	33.7	33.4	-0.3
3	585.3178	585.3185	-0.7	7.2	7.7	0.5

x10⁴ Cpd 1: C30 H48 O11: -ESI Scan (0.6-0.7 min, 5 Scans) Frag=150.0V 241217_3145.d Subtract

m/z	Abund
583.3124	100
584.3158	33.41
585.3185	7.66
586.3212	1.32
587.3237	0.19
588.3263	0.02
589.3288	0

m/z	Abund
565.3	254.77
581.3	225.92
583.31	16757.13
584.32	5648.83
585.32	1207.1
586.32	221.96
651.3	149.83

