

CERTIFICATE of ANALYSIS



Deuterated Bile Acids MaxSpec[®] Discovery Mixture

Item No.:	33506
Batch No.:	0700993
Expiry Date:	22FEB2029 (valid from date of certification)
Supplied as:	A solution in methanol; in a deactivated glass ampule
Verified Concentration:	See table
Volume per Ampule:	Not less than 1 ml. Ampules are overfilled. It is advised that labs use measured volumes.
Storage & Handling:	Store upright and unopened at -20°C. Warm to room temperature prior to opening. Light sensitive.

Description

MaxSpec[®] products are purpose built for mass spectrometry and related applications where quantitative reproducibility is required. This formulated solution has been prepared gravimetrically and is supplied in a deactivated glass ampule sealed under argon. The concentration was verified by comparison to an independently prepared calibration standard. Ongoing stability tests are performed to ensure the concentration remains accurate throughout the shelf life of the product. Follow recommended storage and handling conditions to maintain product quality.

Quality Information

Test	Limit	Result	Meets Specification
Identity, LC-MS	Identities confirmed	Pass	✓
Assay	90 – 110%	See table	✓

Approval:

Title: Manager, Analytical Chemistry

Certification Date: 22FEB2024

Cayman Chemical certifies that this product meets the specifications stated in this certificate and warrants this product to meet the stated acceptance criteria through the expiry date when stored unopened as recommended.

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Quality Control Table

Raw Material Item No.	Raw Material Batch No.	Item Name	Monoisotopic Mass (Da)	Final Conc. (μM)	RT (min)	Assay (%)
31348	0602229	Cholic acid-d ₄	412.3	1.15	3.7	101.3
31350	0591713	Deoxycholic acid-d ₄	396.3	1.65	5.0	96.3
31352	0591716	Glycocholic acid-d ₄	469.3	1.15	3.6	96.1
31354	0591720	Lithocholic acid-d ₄	380.3	0.25	5.9	102.0
31362	0603410	Taurochenodeoxycholic acid-d ₄	503.3	1.00	4.6	98.3
31364	0603314	Glycochenodeoxycholic acid-d ₄	453.3	3.80	4.6	93.0
31366	0602227	Chenodeoxycholic acid-d ₄	396.3	1.15	4.7	98.9
31368	0592200	Ursodeoxycholic acid-d ₄	396.3	0.30	3.0	100.1
31375	0603402	Taurocholic acid-d ₄	519.3	1.00	3.6	97.7
31553	0600807	Glycodeoxycholic acid-d ₄	453.3	1.28	4.9	101.9
31554	0600809	Glycolithocholic-acid-d ₄	437.3	0.25	5.8	93.0
31555	0607164	Glycoursodeoxycholic acid-d ₄	453.3	0.60	2.9	96.3
31563	0607166	Taurodeoxycholic acid-d ₄	503.3	1.00	4.9	96.2
31564	0607169	Tauroursodeoxycholic acid-d ₄	503.3	0.50	2.9	102.3
31571	0607711	Taurolithocholic acid-d ₄	487.3	0.25	5.7	100.5
LC-MS Conditions: Sciex Exion LC-6500 Triple Quadrupole Mass Spectrometer						
Mobile Phase A: Methanol/Water (1:9 v/v) with 10 mM ammonium acetate (+1 ml 25% ammonium hydroxide)						
Mobile Phase B: Methanol with 10 mM ammonium acetate (+1 ml 25% ammonium hydroxide)						
Column: Waters BEH C18 2.1 x 50 mm, 1.7 μm					Oven Temp.: 50°C	
Gradient: 0 min 20%B; 0.2 min 50% B; 6 min 75%B; 7 min 100% B; 8 min 100%B; 8.1 min 20%B; 10 min 20%B						
Injection Volume: 5 μl			Negative Electrospray Ionization		MRM or SIM	

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Stability

Stability testing is ongoing to ensure concentration accuracy. The certificate of analysis and product expiry date will be updated upon completion of testing.

Date	Limit	Result	Meets Specification
22FEB2024	90 – 110%	Pass	✓

Revision History

Revision No.	Date	Reason for Revision
01	22AFEB2024	Initial version
02	09APR2025	Expiry date extension

Disclaimers

Material Safety Data

This material should be considered hazardous until information to the contrary becomes available. Do not ingest, swallow, or inhale. Do not get in eyes, on skin, or on clothing. Wash thoroughly after handling. This information contains some but not all of the information required for the safe and proper use of this material. Before use, review the complete Material Safety Data Sheet, which has been sent *via* email to your institution.

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