

# CERTIFICATE of ANALYSIS



## Deuterated Bile Acids MaxSpec<sup>®</sup> Discovery Mixture

Item No.:	33506
Batch No.:	0608052
Expiry Date:	02FEB2022 (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<sup>®</sup> 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: Director of Analytical Chemistry

Certification Date: 02FEB2021

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	FW (g/mol)	Final Conc. (µM)	RT (min)	Assay (%)
31564	0607169	Tauroursodeoxycholic Acid-d <sub>4</sub>	503.7	0.050	2.7	103
31555	0607164	Glycoursodeoxycholic Acid-d <sub>4</sub>	453.7	0.60	2.7	106
31368	0592200	Ursodeoxycholic Acid-d <sub>4</sub>	396.6	0.30	2.8	106
31375	0603402	Taurocholic Acid-d <sub>4</sub>	519.7	0.175	3.3	93.9
31352	0591716	Glycocholic Acid-d <sub>4</sub>	469.7	1.15	3.3	102
31348	0602229	Cholic Acid-d <sub>4</sub>	412.6	1.15	3.4	97.6
31362	0603410	Taurochenodeoxycholic Acid-d <sub>4</sub>	503.7	0.575	4.3	104
31364	0603314	Glycochenodeoxycholic Acid-d <sub>4</sub>	453.7	3.8	4.4	98.1
31366	0602227	Chenodeoxycholic Acid-d <sub>4</sub>	396.6	1.15	4.5	101
31563	0607166	Taurodeoxycholic Acid-d <sub>4</sub>	503.7	0.20	4.6	108
31553	0600807	Glycodeoxycholic Acid-d <sub>4</sub>	453.7	1.275	4.6	102
31350	0591713	Deoxycholic Acid-d <sub>4</sub>	396.6	1.65	4.7	100
31571	0607711	Tauroolithocholic Acid-d <sub>4</sub>	487.7	0.050	5.5	108
31554	0600809	Glycolithocholic Acid-d <sub>4</sub>	437.7	0.25	5.6	102
31354	0591720	Lithocholic Acid-d <sub>4</sub>	380.6	0.25	5.8	92.2
<b>LC-MS Conditions: Sciex Exion LC-6500 Triple Quadrupole Mass Spectrometer</b>						
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			Flow Rate: 0.4 ml/min		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
02FEB2021	90 - 110%	Pass	✓

## Revision History

Revision No.	Date	Reason for Revision
01	02FEB2021	Initial version

## 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.

### Warranty and Limitation of Remedy

Cayman Chemical Company makes no warranty or guarantee of any kind, whether written or oral, expressed or implied, including without limitation, any warranty of fitness for a particular purpose, suitability and merchantability, which extends beyond the description of the chemicals hereof. Cayman warrants only to the original customer that the material will meet our specifications at the time of delivery.

Cayman will carry out its delivery obligations with due care and skill. Thus, in no event will Cayman have any obligation or liability, whether in tort (including negligence) or in contract, for any direct, indirect, incidental or consequential damages, even if Cayman is informed about their possible existence.

This limitation of liability does not apply in the case of intentional acts or negligence of Cayman, its directors or its employees.

Buyer's exclusive remedy and Cayman's sole liability hereunder shall be limited to a refund of the purchase price, or at Cayman's option, the replacement, at no cost to Buyer, of all material that does not meet our specification.

Said refund or replacement is conditioned on Buyer giving written notice to Cayman within thirty (30) days after arrival of the material at its destination. Failure of Buyer to give said notice within thirty (30) days shall constitute a waiver of Buyer of all claims hereunder with respect to said material.

For further details, please refer to our Warranty and Limitations of Remedy located on our website and in our catalog.

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**CAYMAN CHEMICAL**  
1180 EAST ELLSWORTH RD  
ANN ARBOR, MI 48108 · USA

**PHONE:** [800] 364-9897  
[734] 971-3335  
**FAX:** [734] 971-3640

techserv@caymanchem.com  
www.caymanchem.com