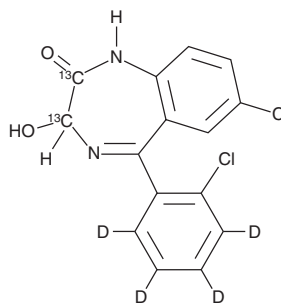


Certified Reference Material



ACCREDITED
ISO 17034 #AR-1774



ANAB
ANSI National Accreditation Board
ACCREDITED
ISO 17034
REFERENCE MATERIAL
PRODUCER

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CRM Assay

Method Parameters	
Cayman Method	TST SD99
Column	4.6 x 150 mm, 5 µm Luna Phenyl-Hexyl
Mobile Phase	A: 10:90:10 mM Acetonitrile:Water:Ammonium Formate B: 90:10:10 mM Acetonitrile:Water:Ammonium Formate
Gradient	<i>Time (min)</i> <i>%B</i> 0-10 31.2-100% 10-13 100% 13.1-20 31.2%
Flow Rate	1 ml/min
Column Temp	30°C
Wavelength	UV monitored at 254 nm

Homogeneity

A minimum sample size of 0.1 µg was used to determine homogeneity. Homogeneity was determined by HPLC using ampules selected from a random sampling plan from early, middle, and late fill positions.

%RSD	Acceptance Criteria
0.91%	≤3%

The recommended minimum quantity for use is 0.1 µg. Quantities below this have not been evaluated.

Neat Material Quality Information (Item No.: 17965, Batch No.: 0583590)

Qualifier	Method	Result
Chromatographic Purity, HPLC	Cayman Method TST SD99	>99.90%
Identity, LC-MS	Cayman Method TST SD13, +ESI	327.0 amu
Identity, GC-MS	Cayman Method TST SD12	Conforms
Identity, FTIR	Cayman Method TST SD03	Conforms
% LOD	Cayman Method TST SD24	0.20%
% ROI	Cayman Method TST SD06	<0.10%
Isotopic Purity, LC-MS	Cayman Method TST SD154	<0.10% M ₀ vs. M ₆
Identity, NMR	¹ H NMR	Conforms

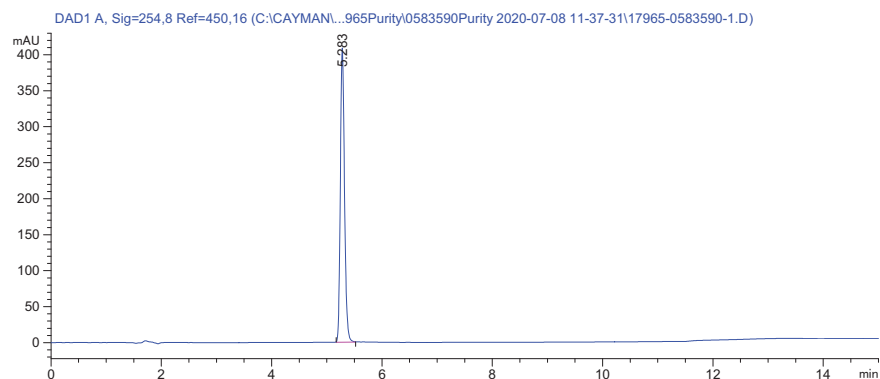
NMR and optical rotation (if applicable) are provided as supplemental information but are not within scope of ISO accreditation. Property values are traceable to SI units through an unbroken chain of measurements.

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Supplemental Data (Neat Material)

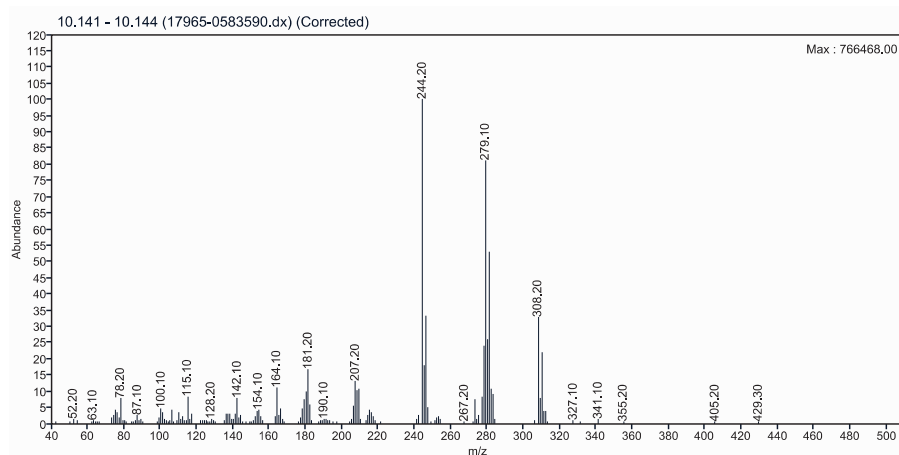
HPLC-UV



Conditions

Instrument	Agilent 1100/1200 Series								
Column	4.6 x 150 mm, 5 µm Luna Phenyl-Hexyl								
Mobile Phase	A: 10:90:10 mM Acetonitrile: Water:Ammonium Formate B: 90:10:10 mM Acetonitrile: Water:Ammonium Formate								
Gradient	<table border="1"> <thead> <tr> <th>Time (min)</th> <th>%B</th> </tr> </thead> <tbody> <tr> <td>0-10</td> <td>31.2-100%</td> </tr> <tr> <td>10-13</td> <td>100%</td> </tr> <tr> <td>13.1-20</td> <td>31.2%</td> </tr> </tbody> </table>	Time (min)	%B	0-10	31.2-100%	10-13	100%	13.1-20	31.2%
Time (min)	%B								
0-10	31.2-100%								
10-13	100%								
13.1-20	31.2%								
Flow Rate	1 ml/min								
Column Temp	30°C								
Wavelength	UV monitored at 254 nm								

GC-MS



Conditions

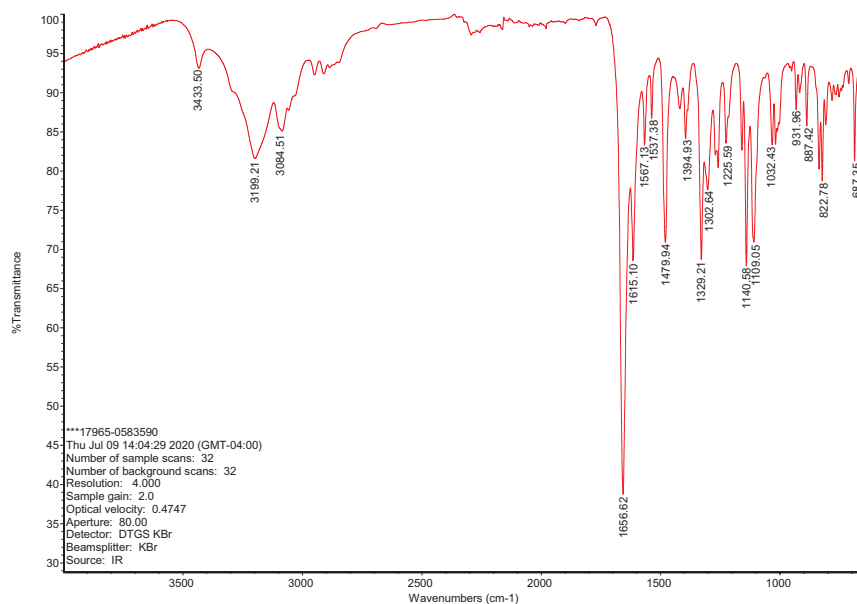
Instrument	Agilent GC MSD
Column	30 m x 0.32 mm, 0.5 µm Rtx-5MS
Carrier Gas	He
Flow Rate	2 ml/min
Inlet Temp	300°C
Split Ratio	15:1
Oven Program	50°C hold for 1 min, ramp to 300°C at 30°C per min, hold at 300°C to 15 min
Transfer Line Temp	300°C
Voltage	70eV EI MS
Scan Range	40-650 m/z
Tune File	etune

Apex spectrum – background (1 min window in front of peak)

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FTIR

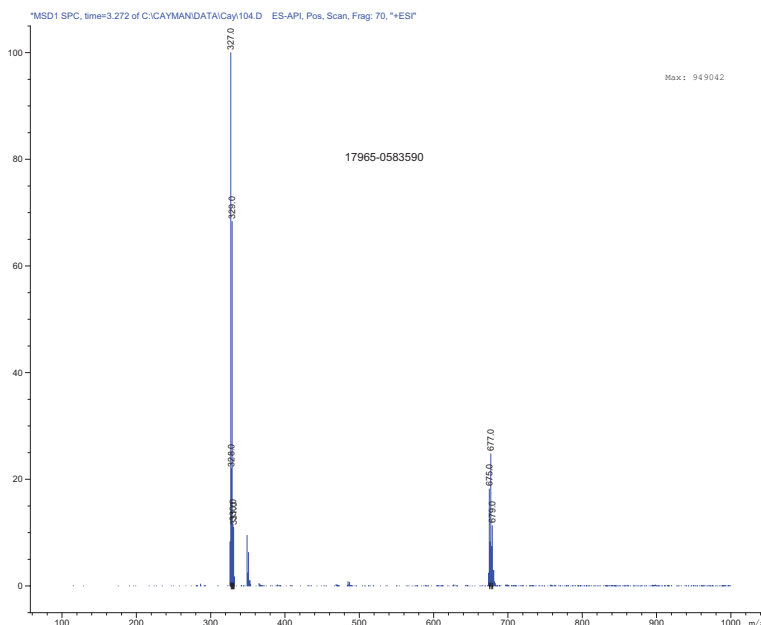


Conditions

Instrument	Thermo Nicolet iS10 FTIR / Diamond SmartATR (single bounce)
Scans	32 scans / 32 background scans
Range	650-4,000 cm ⁻¹
Resolution	4.000

ATR and background corrected

ESI-MS



Conditions

Instrument	Agilent HPLC MSD
Mobile Phase	50:50:0.1 methanol/water/acetic acid
Flow Rate	0.5 ml/min
Ionization Mode	+ESI
Mass Range	100-1,000 m/z
Nebulizer	60 psi
Desolvation Gas	13 L/min
Desolvation Temp	350°C
Electrospray Voltage	4kV

MS collected across peak width at half height

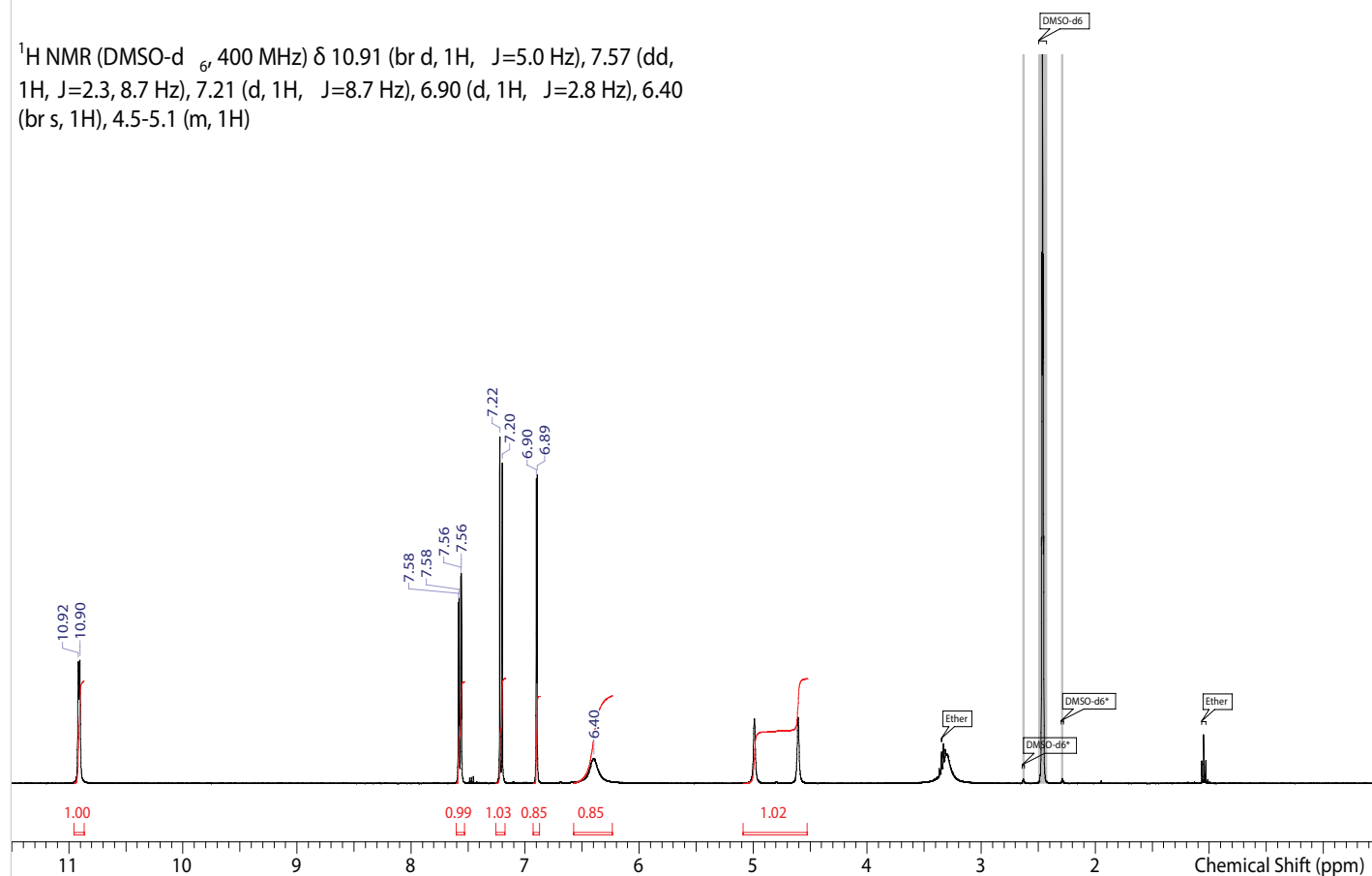
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NMR (not within scope of ISO accreditation)

File Name	\\sulfur\private\nmrdata\JEOL_2020\YL-1917-227-1_PROTON_02-Jul-2020-1-1.jdf		
Date	02 Jul 2020 13:07:26	Nucleus	¹ H
Solvent	DMSO-d ₆	Frequency (MHz)	399.7822
		Number of Transients	16
		Temperature (degree C)	20.700

¹H NMR (DMSO-d₆, 400 MHz) δ 10.91 (br d, 1H, J=5.0 Hz), 7.57 (dd, 1H, J=2.3, 8.7 Hz), 7.21 (d, 1H, J=8.7 Hz), 6.90 (d, 1H, J=2.8 Hz), 6.40 (br s, 1H), 4.5-5.1 (m, 1H)



Conditions

Instrument	JEOL ECZ 400S
Scans	16 scans

Stability

The effect of the components of stability on the combined standard uncertainty of the CRM property value are considered negligible unless indicated in stability studies.

Short-Term Stability

No decrease in the property value was observed at ambient or 60°C after two weeks. This data supports shipping of this product at ambient temperature.

Long-Term Stability

Long-term stability data confirmed five years stability at the -20°C storage temperature.

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Quality Standard Documentation

The manufacturer of this Certified Reference Material is accredited under ISO 17034:2016 accreditation issued by ANAB. Refer to ANAB certificate and scope of accreditation AR-1774.

The manufacturer of this Certified Reference Material is accredited under ISO/IEC 17025:2017 accreditation issued by ANAB. Refer to the ANAB certificate and scope of accreditation AT-1773.

Revision History

Revision No.	Date	Reason for Revision
01	03APR2024	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 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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ISO CRT SD02 v 5.1

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