

Certificate of Analysis

Reference Material

Product name

4-(4-Hydroxy-3-iodophenoxy)-3,5-diiodobenzoic Acid
(3,3',5-Triiodothyroformic Acid)

Product code

MM0694.16-0025

CAS number

4618-45-5

Molecular weight

607.91

Molecular formula

C₁₃H₇I₃O₄

Lot number

1150970

Appearance

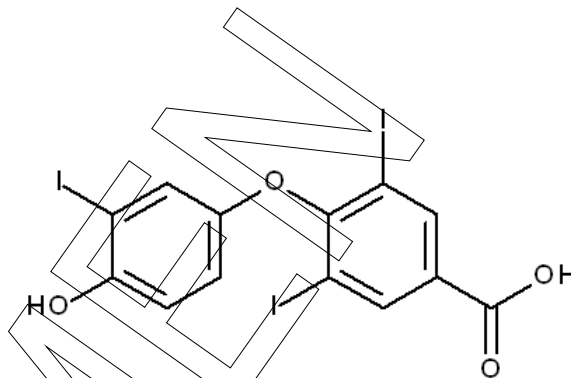
off-white solid

Melting point (DSC)

264 °C

Long-term storage

2 to 8 °C, dark



Assay "as is"
97.3 %

Date of shipment:

09 Sep 2022

Producer confirms that this reference material (RM) meets the specification detailed on this Certificate of Analysis for **one year** from the date of shipment, provided the substance is stored under the recommended conditions unopened in the original container.

Release by:	Date of Release:		Product Release
Dr. Sabine Schröder	Luckenwalde, 10 Aug 2021		



MikromolTM

Product information

For laboratory use only. Not suitable for human or animal consumption.

Before usage of the RM, it should be allowed to warm to room temperature. No drying required, as the certified value is already corrected for the content of water and other volatile materials.

The product quality is controlled by regularly performed quality control tests (retests).

Further content

Identity

Assay

Final result

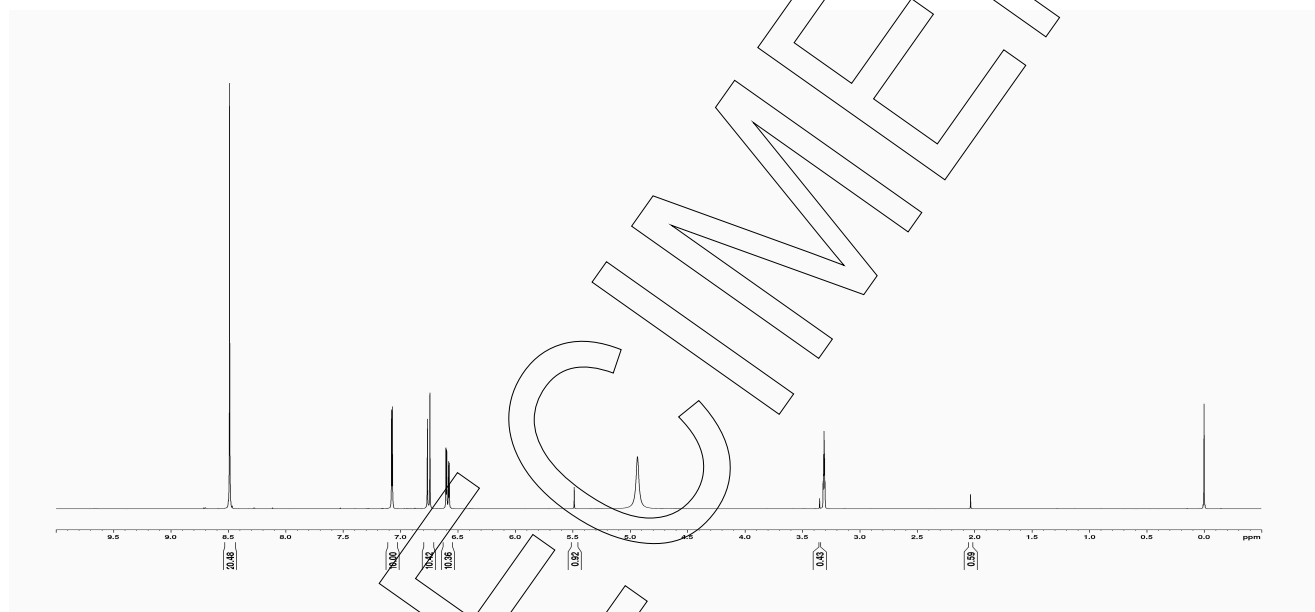
Revision table

SPECIMEN

Identity

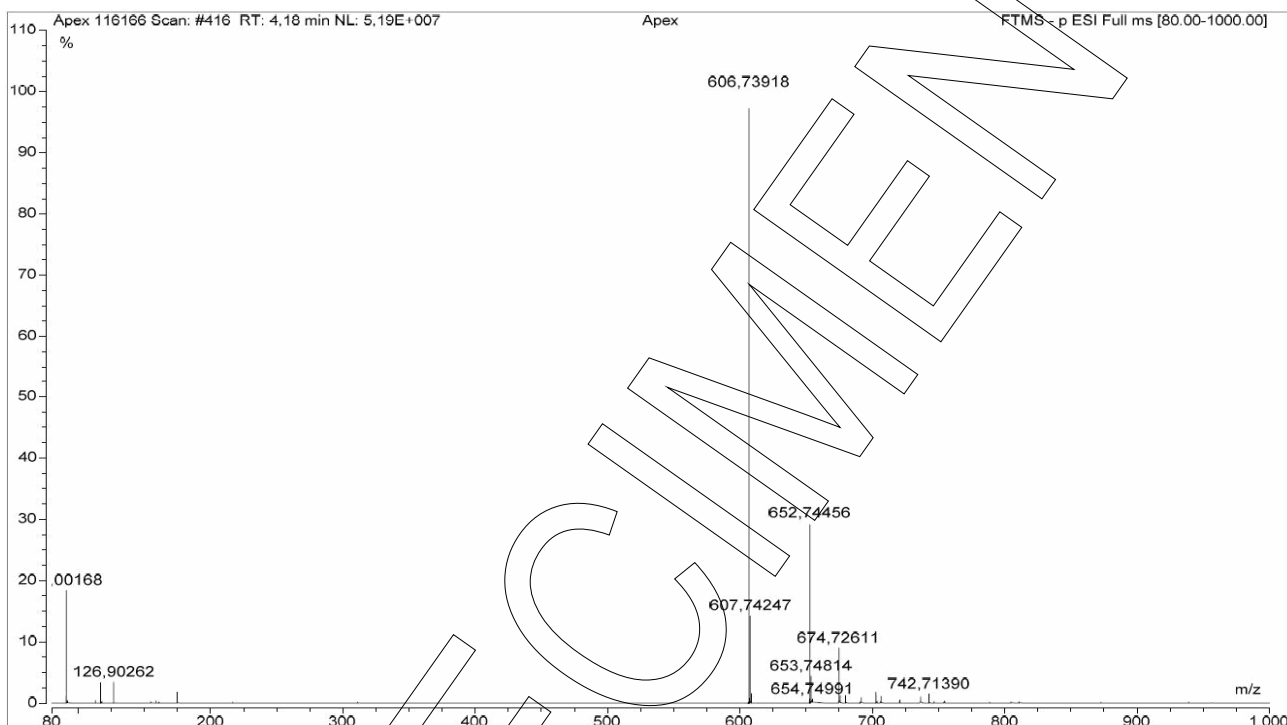
The identity of the reference material was established by following analyses.

Method	Conditions	Result
$^1\text{H-NMR}$	400 MHz, CD_3OD	Structure confirmed



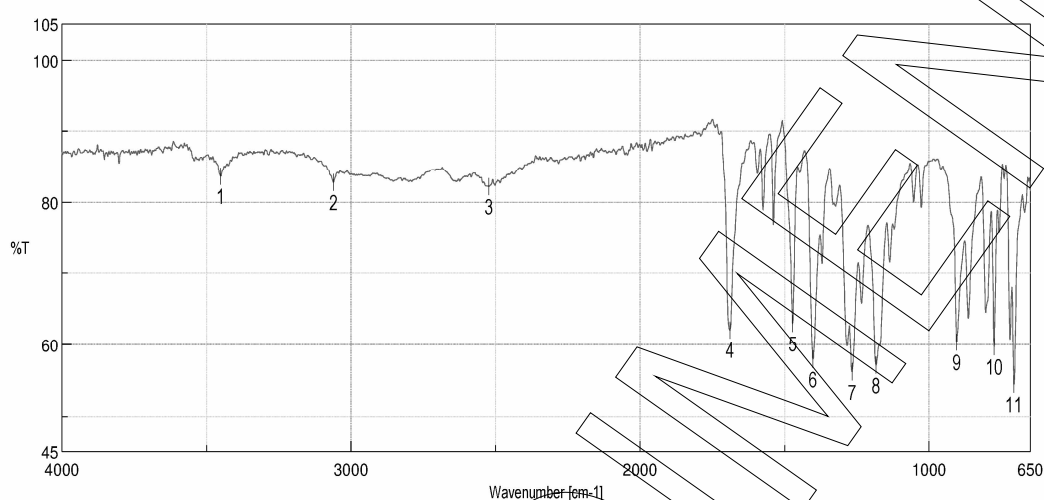


Method	Conditions	Result
MS	3.2 kV ESI-; capillary temperature: 269 °C Theoretical value: 606.74056	Structure confirmed





Method	Conditions	Result
IR	Attenuated Total Reflection Fourier Transform Infrared (ATR-FTIR) Spectroscopy	Structure confirmed



Results of Peak Find

No.	Position	Intensity
1	3450.99	83.5839
2	3061.44	82.7337
3	2523.4	82.1339
4	1689.34	61.9886
5	1472.38	62.9024
6	1402	57.8895
7	1267	56.1284
8	1184.08	57.0692
9	905.415	60.2866
10	775.244	59.6397
11	706.783	54.4239

SPECIMEN



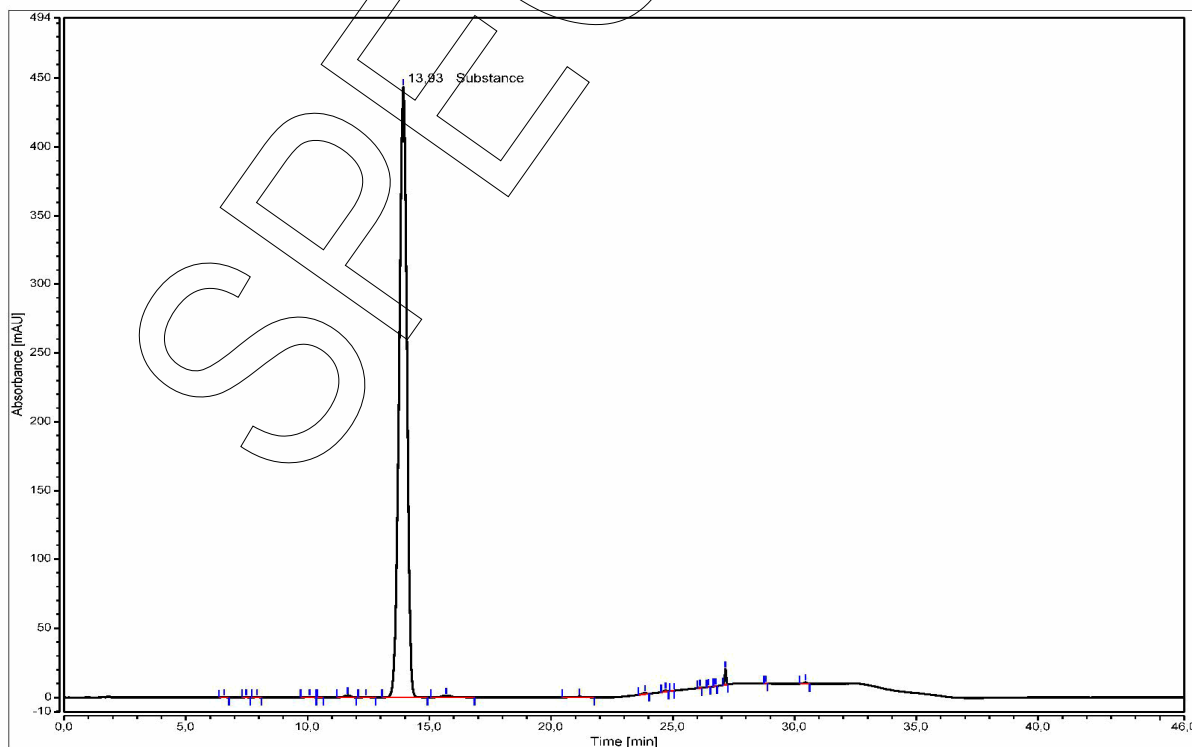
Assay

The assay of the reference material was assessed by following analyses.

Purity by high performance liquid chromatography (HPLC)

HPLC Conditions:	
Column	Hypersil Gold C18; 5 µm, 150 x 4.6 mm
Column temperature	40 °C
Detector	DAD, 230 nm
Injector	Auto 2 µl; 0.2436 mg/ml in Acetonitrile/Water 50/50 (v/v)
Flow rate	1.0 ml/min
Phase A	Water, 0.1 % H ₃ PO ₄
Phase B	Acetonitrile, 0.1 % H ₃ PO ₄
Gradient program	0-20 min A/B 58/42 20-25 min A/B to 20/80 25-30 min A/B 20/80 30-34 min A/B to 58/42 34-46 min A/B 58/42 (v/v)

HPLC chromatogram and peak table





Area percent report - sorted by signal

Pk #	Retention time	Area	Area %	
1	6.567	0.0633	0.04	
2	7.473	0.0159	0.01	
3	7.915	0.0329	0.02	
4	10.078	0.1194	0.07	
5	10.400	0.0103	0.01	
6	11.643	0.4515	0.27	
7	12.398	0.0566	0.03	
8	13.930	163.6134	98.22	
9	15.690	0.6464	0.39	
10	21.160	0.2696	0.16	
11	23.852	0.2043	0.12	
12	24.698	0.1159	0.07	
13	25.058	0.0095	0.01	
14	26.107	0.0255	0.02	
15	26.465	0.0214	0.01	
16	26.755	0.0112	0.01	
17	27.155	0.7567	0.45	
18	28.812	0.0109	0.01	
19	30.443	0.1505	0.09	
Totals		166.5852	100.00	

The content of the analyte was determined as ratio of the peak area of the analyte and the cumulative areas of the purities, added up to 100 %. System peaks were ignored in calculation.



Result (n = 3)

98.22 %; SD < 0.01 %

Volatile content

Water content

Method	Karl Fischer titration
Result (n = 3)	0.11 %; SD = 0.02 %

Residual solvents

Method	¹ H-NMR
Result (n = 1)	Sum: 0.80 % 0.12 % Acetonitrile; 0.06 % Methanol 0.62 % Methylene chloride

Final result

Assay "as is": 97.33 %

The assay "as is" is assessed by 100% method (mass balance) and is equivalent to the assay based on the not anhydrous and not dried substance respectively.

The calculation of the 100% method follows the formula:

$$\text{Assay (\%)} = (100\% - \text{volatile contents (\%)}) * \frac{\text{Purity (\%)}}{100\%}$$

Volatile contents are considered as absolute contributions and purity is considered as relative contribution. Inorganic residues are excluded by additional tests.

Revision table

Revision	Date	Reason for revision
00	10 Aug 2021	Release of the Certificate of Analysis - initial version

Product warranties for the RM are set out in the terms and conditions of purchase.