





Instructions for Use

fleXstandard Polymers

PMMA mixture for calibration of matrix-assisted laser desorption and ionization time-of-flight mass spectrometers (MALDI-TOF MS)

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Product Description

fleXstandard Polymers is a mixture for the calibration of matrix-assisted laser desorption and ionization time-of-flight mass spectrometers (MALDI-TOF MS) for polymer applications. It allows calibrations (15 x 250 calibration points) and testing of MALDI-TOF mass spectrometers in a mass range between ~300 and 10,000 Da. The mixture contains distributions of three different PMMA standards. A selection of the compounds is listed in the following table together with their molecular weights.

The standard is for research use only. It is not for use in diagnostic procedures.

Oligomer	[M+Na] ⁺ Monoisotopic	[M+Na] ⁺ Average
H(C ₅ H ₈ O ₂) ₄ H	425.2146	425.48
H(C ₅ H ₈ O ₂) ₁₄ H	1425.7389	1426.63
H(C ₅ H ₈ O ₂) ₂₄ H	2426.2632	2427.79
H(C ₅ H ₈ O ₂) ₃₄ H	3426.7875	3428.95
H(C ₅ H ₈ O ₂) ₄₄ H	4427.3118	4430.11
H(C ₅ H ₈ O ₂) ₅₄ H	5427.8361	5431.27
H(C ₅ H ₈ O ₂) ₆₄ H	6428.3604	6432.43
H(C ₅ H ₈ O ₂) ₇₄ H	7428.8847	7433.59
H(C ₅ H ₈ O ₂) ₈₄ H	8429.4090	8434.75
H(C ₅ H ₈ O ₂) ₉₄ H	9429.9332	9435.91

Table 2-1	Calibrant oligomers together with their [M+Na]+ m/z values
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Ordering Information

Product	Part Number
fleXstandard Polymers, 15 tubes	# 1880825

This kit is for research use only. Not for use in clinical diagnostic procedures.

Storage and Stability

fleXstandard Polymers is shipped at ambient temperature. We recommend storing fleXstandard Polymers on arrival at room temperature in the dark.

Dissolved samples should be kept in the dark at room temperature for up to two weeks. We do not recommend freezing dissolved samples.

Risk and Safety Information

fleXstandard Polymers is not classified according to Regulation (EC) No. 1272/2008 and is, therefore, not classified according to the Globally Harmonized System of Classification and Labeling of Chemicals (GHS). In the manufacturer's experience, the product has no harmful effect when used and handled according to specifications.

For more information, read the Safety Data Sheet available for download at www.bruker.com/care.

Additional chemicals may be required for procedures described in these Instructions for Use. Carefully read the Safety Data Sheet provided by the supplier and follow general safety regulations when handling chemicals or biohazardous material.

The following chemicals are used in the preparation procedures:



WARNING

DCTB is harmful (H302, H312, H332).

WARNING

Tetrahydrofuran is highly flammable and harmful (H: H225-H302+H319+H335-H351).

1 Sample Preparation Procedure (recommendation)

1.1 Preliminary remarks

Poor sample preparation will degrade sensitivity, yield low resolution and poor reproducibility. The generation of ions through MALDI depends on the production of a suitable composite material, consisting of the matrix substance and the analyte. For best results use only chemicals of highest purity available.

1.1.1 Chemicals and materials required

- trans-2-[3-(4-tert-Butylphenyl)-2-methyl-2-propenylidene]malononitrile (DCTB)
- Sodium trifluoroacetate (NaTFA)
- Tetrahydrofuran (THF)
- Brown autosampler glass vials 2 mL with screw cap and Teflon septum
- Eppendorf Safe-Lock microcentrifuge tubes 0.5 mL
- MALDI ground steel target plate

1.1.2 Equipment and tools required

- Vortex mixer or shaker
- Pipettes and pipette tips

1.2 Preparation of fleXstandard Polymers solution

Dissolve the content of one tube of fleXstandard Polymers in 500 µL THF solvent and vortex/shake for several seconds.

1.3 Preparation of DCTB and NaTFA solution

Use brown autosampler glass vials 2 mL with screw cap and Teflon septum for the preparation of these solutions.

Dissolve DTCB in THF solvent at a concentration of 20 g/L. NaTFA should be dissolved at 0.1 M (13.6 g/L) in THF. Vortex/shake both solutions for several seconds.

1.4 Preparation of a sample onto a MALDI target plate

Use the lid of an open 0.5 mL microcentrifuge tube for mixing. First add 50 μ L of the matrix solution followed by 2 μ L of fleXstandard Polymers solution and 2 μ L NaTFA solution. Always pipet up and down at least 3 times when adding the 2 μ L volumes.

Apply 1 μ L of this mixture onto ~ four spots of a standard ground steel MALDI target plate. Place the pipet tip on the surface of the target plate and slowly drag it over the surface. Do not try to keep the droplet at one position of the target plate as this might result in an inhomogeneous sample preparation.

1.5 Calibration

For a calibration of the flexControl method the MassControlList FleXstandard_Polymer_Na_ mono.mcl should be used for isotopically resolved spectra, while spectra obtained in the linear operation mode of the instrument should be calibrated using the FleXstandard_Polymer_Na_ avg.mcl MassContolList.

A calibration in flexAnalysis can be performed using the CalibratePolymerStandard_ mono.FAMSMethod or CalibratePolymerStandard_avg.FAMSMethod in reflector and linear mode. In case these methods are not yet available on your computer, please contact Polymer.Support.MS@bruker.com.

2 Result of Measurement of fleXstandard Polymers

fleXstandard Polymers is tested on a Bruker ultrafleXtreme MALDI-TOF mass spectrometer. Figure 2-1 shows a typical MALDI-TOF mass spectrum of fleXstandard Polymers obtained from a MALDI target preparation with DCTB matrix and NaTFA as ionizing agent.

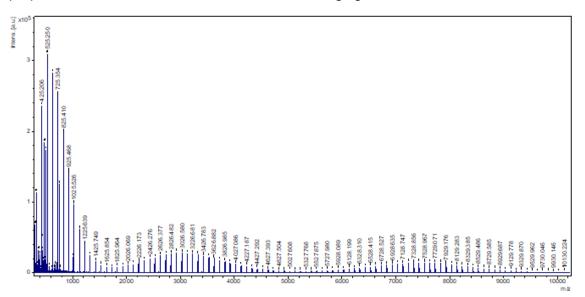


Figure 2-1 MALDI-TOF mass spectrum of fleXstandard Polymers

Symbols

The following symbols are used in the labeling:

REF	Catalogue number
RUO	Research Use Only
	General warning
*	Flammable warning
	Aspiration hazard warning
	Manufacturer
	Temperature limit
LOT	Batch code
	Use-by date
i	Consult instructions for use

Manufacturer



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For research use only. Not for use in clinical diagnostic procedures.

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