

SpheriCal® for IM-MS calibration

Thank you for purchasing SpheriCal® for IM-MS.

SpheriCal® IM-MS Low Range is a mixture of 10 different dendritic components that cover the following ranges within m/z , CCS, and charge states:

Mode	Molecular masses [Da]	m/z *		CCS _{N2} range * [Å ²]	Charge states *
positive ESI	294 – 1,893	[M+nNa] ⁿ⁺	317 – 1,915	160 – 438	+1; +2
		[M+nH] ⁿ⁺	295 – 1,894	180 - 408	+1; +2
positive MALDI	294 – 1,893	[M+Na] ⁺	317 – 1,915	160 – 412	+1
negative ESI	294 – 1,893	[M-H] ⁿ⁻	293 – 1,892	tbd	-1; -2
		[M+FA-nH] ⁿ⁻	339 – 1,938	tbd	-1; -2
		[M+TFA-nH] ⁿ⁻	407 - 2,006	tbd	-1; -2

* Observable ions and charge states depend on instrumentation, sample preparation and ionization conditions.

1. Product Description and Storage Information

SpheriCal® IM-MS Low Range is a mixture of ten monodisperse dendrimers which are intended for m/z and CCS calibration and tuning of IM-MS instrumentation.

1.1. Storage and shelf life

SpheriCal® is shipped without temperature control. Once received, please store the vials in the freezer at -20°C to ensure a shelf life of 3 years post production. The expiring date is stated on each vial.

Chemically, the SpheriCal® technology can be considered a polyester. As such, the molecules are very stable over a long period of time. However, hydrolysis can occur in aqueous environments at highly acidic or highly basic conditions. Accordingly, we advise you to store SpheriCal® in dry conditions in the freezer prior to use. Once aqueous aliquots are prepared, it is crucial to store them in the freezer.

2. Instructions for Usage

2.1. Preparation of ESI spraying solution

The product is soluble in polar solvents, such as methanol, ethanol, THF and aqueous mixtures of these, as well as aqueous acetonitrile. For aqueous acetonitrile, we recommend mixing the solvents first before adding the mixture to the product vial. The products have been developed based on 50/50 ACN/H₂O v/v. For negative mode, add small amounts of formic acid, acetic acid or tri-fluoro acetic acid (0.1% of the aqueous portion).

Simply add 1.00 mL of spraying solution the product vials and shake well or use a vortex mixer. Prepare aliquots that match your intended/expected use in suitable vials and store in the freezer. Prevent repeated thawing/freezing of the aliquots.

2.2. Preparation of MALDI spots

- Pre-spot the desired position with 0.5 μ L of NaTFA solution at 2 mg/mL.
- Add 20 μ L solvent to prepare the SpheriCal solution at 0.5 mg/mL. Add 0.5 μ L onto the desired spot and let dry.
- Prepare the matrix solution at 20 mg/mL and add 0.5 μ L on top of the NaTFA/SpheriCal and let dry.
- Suitable matrices are HCCA, DHB, graphite.

3. Observable ions and their parameters

3.1. Composition

SpheriCal[®] IM-MS consists of ten dendritic components that cover a molecular mass between 294 and 1,893 Da, see Table 1.

Table 1. Components of SpheriCal[®] IM-MS Low Range

Component ID	Chemical Formula	M_{mono} [Da]
PFS-1022	C ₁₂ H ₂₂ O ₈	294.131
PFS-2012	C ₁₇ H ₃₀ O ₁₀	394.184
PFS-1032	C ₂₀ H ₃₆ O ₁₂	468.221
PFS-1042	C ₂₅ H ₄₄ O ₁₆	600.263
PFS-1052	C ₃₀ H ₅₂ O ₂₀	732.305
PFS-3012	C ₃₇ H ₆₂ O ₂₂	858.373
PFS-1062	C ₄₀ H ₇₀ O ₂₅	950.421
PFS-2032	C ₅₀ H ₈₄ O ₃₀	1164.505
PFS-2042	C ₆₅ H ₁₀₈ O ₄₀	1528.642
PFS-2052	C ₈₀ H ₁₃₂ O ₅₀	1892.779

3.2. Positive mode

In general, the components in the mixture form mostly $[M+nNa]^{n+}$ ions in positive mode. $[M+nH]^{n+}$ might also be observable. Intensity ratios between sodiated and protonated ions are related to the availability of sodium ions during the ionization process. Observable ions are listed in Table 2.

Figure 1 shows an ESI-MS spectrum, Figure 2 shows the MALDI-MS spectrum, and Figure 3 shows the mobility traces of this product.

Table 2. Observable ions of SpheriCal® IM-MS Low Range in positive mode.

Ion	<i>m/z</i>	^{DT} CCS _{N₂} [Å ²]
[PFS-1022+H] ⁺	295.139	tbd
[PFS-1022+Na] ⁺	317.121	160.65
[PFS-2012+H] ⁺	395.191	180.88
[PFS-2012+Na] ⁺	417.173	185.39
[PFS-1032+H] ⁺	469.228	197.50
[PFS-1032+Na] ⁺	491.210	198.51
[PFS-2032+2H] ²⁺	583.260	346.21
[PFS-1042+H] ⁺	601.270	218.56
[PFS-2032+2Na] ²⁺	605.242	351.19
[PFS-1042+Na] ⁺	623.252	220.65
[PFS-1052+H] ⁺	733.312	245.51
[PFS-1052+Na] ⁺	755.294	246.40
[PFS-2042+2H] ²⁺	765.328	386.62
[PFS-2042+2Na] ²⁺	787.310	388.89
[PFS-3012+H] ⁺	859.381	tbd
[PFS-3012+Na] ⁺	881.362	270.24
[PFS-2052+2H] ²⁺	947.397	433.39
[PFS-1062+H] ⁺	951.428	284.51
[PFS-2052+2Na] ²⁺	969.379	438.51
[PFS-1062+Na] ⁺	973.410	287.23
[PFS-2032+H] ⁺	1165.512	315.77
[PFS-2032+Na] ⁺	1187.494	317.41
[PFS-2042+H] ⁺	1529.649	363.02
[PFS-2042+Na] ⁺	1551.631	366.74
[PFS-2052+H] ⁺	1893.786	408.23
[PFS-2052+Na] ⁺	1915.768	411.72

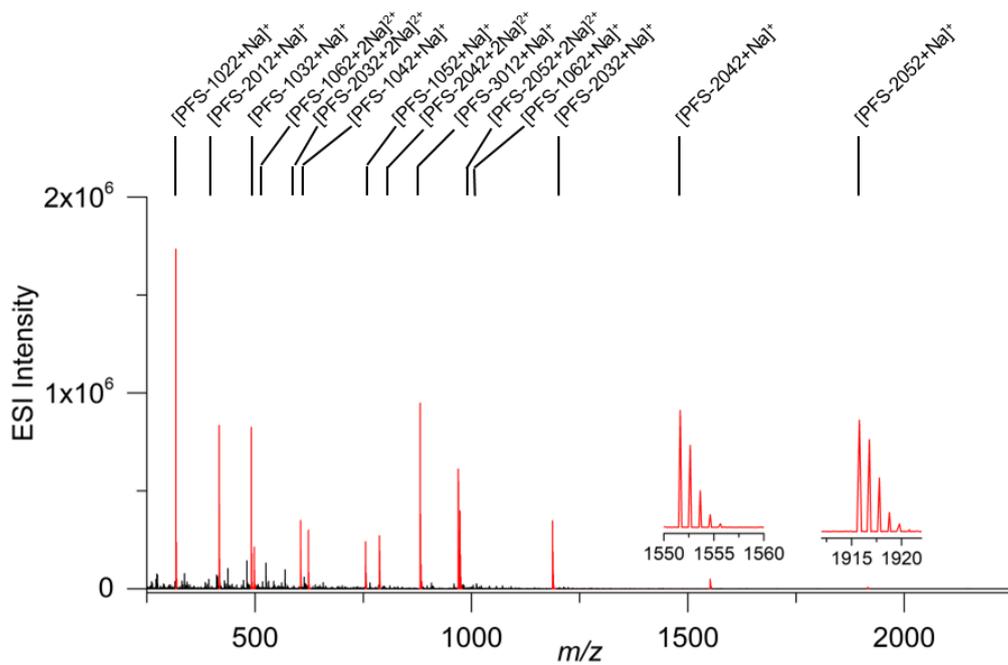


Figure 1: ESI spectrum of SpheriCal[®] IM-MS Low Range in positive mode as measured on a Waters Cyclic IMS from ACN/H₂O/FA 50/49.95/0.05.

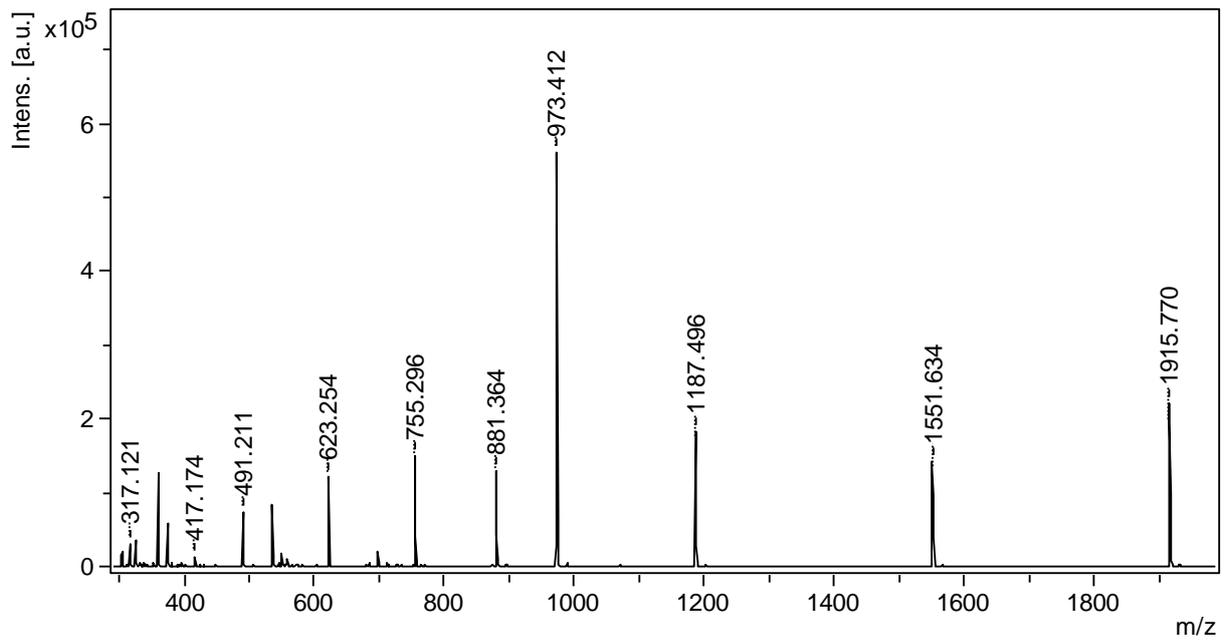


Figure 2: MALDI-MS spectrum of SpheriCal IM-MS Low Range in positive mode, using DHB as matrix.

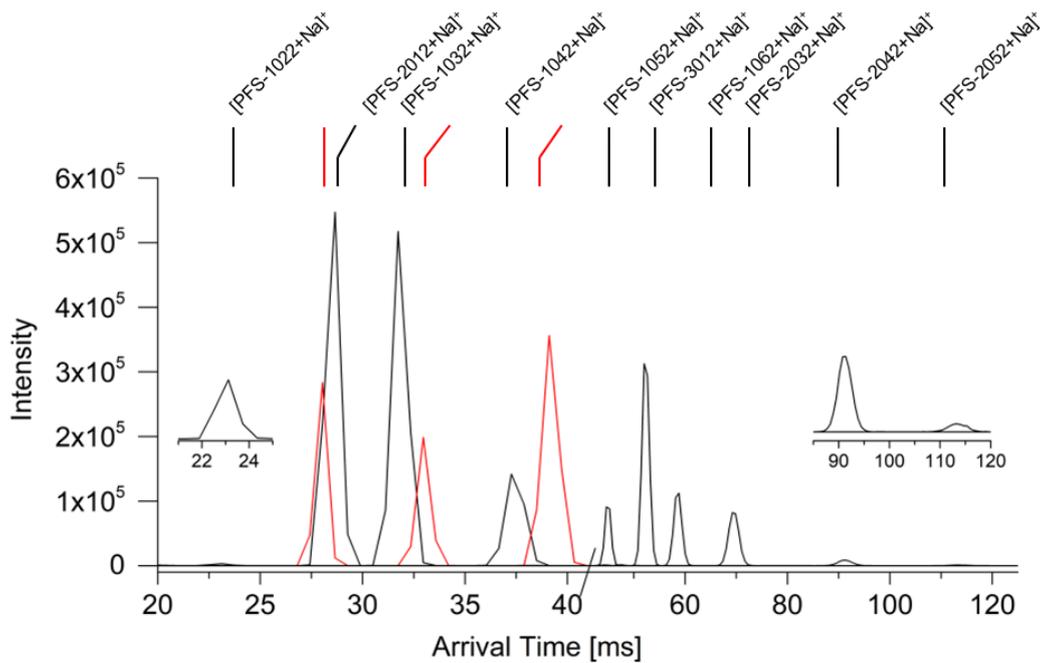


Figure 3. Arrival times for sodiated ions of SpheriCal® IM-MS Low Range as measured on the Waters Cyclic IMS, one cycle.

3.3. Negative mode

Please observe: Negative mode works in ESI, but not in MALDI. No CCS values for the negative ions have been reported yet.

In ESI-MS, the components will form $[M-nH]^{n-}$ and adducts with anions of available acids, such as $[M+nCOOH-nH]^{n-}$ for formic acid. If several acids are available, the components will form various adducts. The combination TFA and FA yield well-spaced signals.

Figure 4 shows an ESI-MS spectrum in negative mode and Table 4 lists observable ions with their m/z .

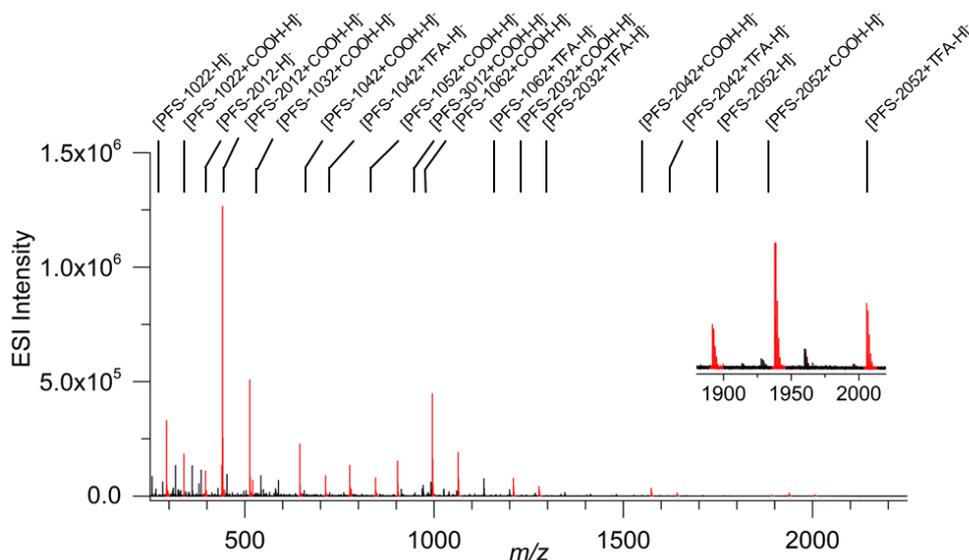


Figure 4: Mass spectrum of SpheriCal® IM-MS Low Range in negative mode as measured on a Waters Cyclic IMS from ACN/H₂O/FA 50/49.95/0.05. Remaining traces of TFA in the used hardware result in additional signals.

Table 4. Observable ions of SpheriCal® IM-MS Low Range in negative mode.

Ion	m/z
[PFS-1022-H] ⁻	293.123
[PFS-1022+COOH-H] ⁻	339.129
[PFS-2012-H] ⁻	393.176
[PFS-1022+TFA-H] ⁻	407.116
[PFS-2012+COOH-H] ⁻	439.181
[PFS-1032-H] ⁻	467.212
[PFS-2012+TFA-H] ⁻	507.168
[PFS-1032+COOH-H] ⁻	513.218
[PFS-1032+TFA-H] ⁻	581.205
[PFS-2032-2H] ²⁻	581.244
[PFS-1042-H] ⁻	599.255
[PFS-2032+2COOH-2H] ²⁻	627.249
[PFS-1042+COOH-H] ⁻	645.260
[PFS-2032+2TFA-2H] ²⁻	695.237
[PFS-1042+TFA-H] ⁻	713.247
[PFS-1052-H] ⁻	731.297
[PFS-2042-2H] ²⁻	763.312
[PFS-1052+COOH-H] ⁻	777.302
[PFS-2042+2COOH-2H] ²⁻	809.318
[PFS-1052+TFA-H] ⁻	845.290
[PFS-3012-H] ⁻	857.365
[PFS-2042+2TFA-2H] ²⁻	877.305
[PFS-3012+COOH-H] ⁻	903.370
[PFS-2052-2H] ²⁻	945.381
[PFS-1062-H] ⁻	949.412
[PFS-3012+TFA-H] ⁻	971.358
[PFS-2052+2COOH-2H] ²⁻	991.386
[PFS-1062+COOH-H] ⁻	995.418
[PFS-2052+2TFA-2H] ²⁻	1059.374
[PFS-1062+TFA-H] ⁻	1063.405
[PFS-2032-H] ⁻	1163.496
[PFS-2032+COOH-H] ⁻	1209.502
[PFS-2032+TFA-H] ⁻	1277.489
[PFS-2042-H] ⁻	1527.633
[PFS-2042+COOH-H] ⁻	1573.639
[PFS-2042+TFA-H] ⁻	1641.626
[PFS-2052-H] ⁻	1891.770
[PFS-2052+COOH-H] ⁻	1937.776
[PFS-2052+TFA-H] ⁻	2005.763

4. Feedback

We hope you are satisfied with the product. We are eager to hear your thoughts on our products and reward shared data and constructive feedback with a discount on your next order. Please reach out to jens.sommertune@polymerfactory.com for more information.

Contact

Please feel free to email any inquiries about SpheriCal® to jens.sommertune@polymerfactory.com.

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