SpheriCal® for tuning and calibration of IM-MS equipment

Thank you for purchasing SpheriCal® for IM-MS.

SpheriCal® IM-MS High Range is a mixture of 9 different dendritic components that ionize both with MALDI and ESI sources. In MALDI, singly charged $[M+Na]^+$ are expected and work in positive mode only. In ESI, both negative and positive mode are working and yield multiple charge states depending on the molecular mass of the dendrimer.

This mixture covers the following ranges within *m/z*, CCS, and charge states:

Mode	Molecular masses [Da]	*m/z**		CCS_{N2} range * [Å²]	Charge states *
ESI positive	1,164 – 18,140	$[M+nNa]^{n+}$ $[M+nH]^{n+}$	605 – 2,615 583 – 2,368	317 – 1,732	+1 → +7
MALDI positive	1,164 – 18,140	$[M+Na]^+$	1,187 – 18,150	317 - tbd	+1
ESI negative	1,164 – 18,140	$[M-H]^{n-}$ $[M+FA-nH]^{n-}$ $[M+TFA-nH]^{n-}$	581 – 3,632 627 – 3,678 695 – 3,746	tbd tbd tbd	-1 → -6 -1 → -6 -1 → -6

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

1. Product Description and Storage Information

SpheriCal® IM-MS High 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/H_2O 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 0.5µL of NaTFA solution at 2 mg/mL.
- Add 20 µL solvent to prepare the SpheriCal solution at 0.5 mg/mL. Add 0.5 µL onto the desired spot and let dry.
- Prepare the matrix solution at 20 mg/mL and att 0.5µL on top of the NaTFA/SpheriCal and let dry.
- Suitable matrices are HCCA and DHB.

3. Observable ions and their parameters

3.1. Composition

SpheriCal® IM-MS consists of nine dendritic components that cover a molecular mass between 1,164 and 18,140 Da, see Table 1.

Table 1. Components of SpheriCal® IM-MS High Range

Component ID	Chemical Formula	M_{mono} [Da]
PFS-2032	$C_{50}H_{84}O_{30}$	1,164.5047
PFS-2052	$C_{80}H_{132}O_{50}$	1,892.7786
PFS-2062	$C_{100}H_{166}O_{61}$	2,342.9887
PFS-3052	$C_{180}H_{292}O_{110}$	4,213.7255
PFS-3062	$C_{220}H_{358}O_{133}$	5,128.1250
PFS-4042	$C_{305}H_{492}O_{184}$	7,098.9142
PFS-4052	$C_{380}H_{612}O_{230}$	8,855.6193
PFS-4062	$C_{460}H_{742}O_{277}$	10,698.3975
PFS-5042	$C_{625}H_{1004}O_{376}$	14,525.9442
PFS-5052	$C_{780}H_{1252}O_{470}$	18,139.4068

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 in ESI. In ESI, 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 along with arrival times, Figure 2 shows the MALDI-MS spectrum.
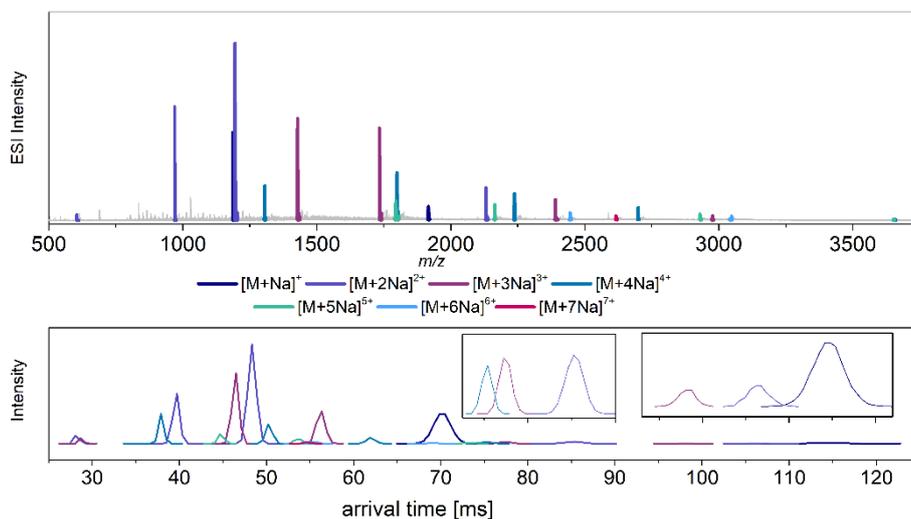

Figure 1: ESI spectrum of SpheriCal® IM-MS High Range in positive mode as measured on a Waters Cyclic IMS from ACN/H_2O/FA 50/49.95/0.05 along with arrival times (1 cycle).
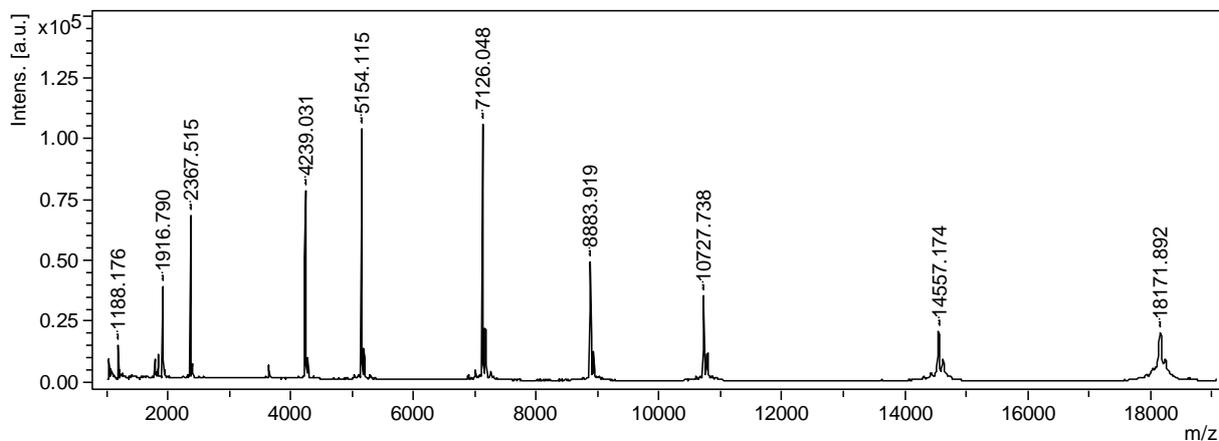
Figure 2: MALDI-MS spectrum of SpheriCal IM-MS High Range in positive mode, using DHB as matrix.

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

Component ID	Chemical Formula	Ion	m/z	$^{DT}CCS_{N2}$
PFS-2032	$C_{50}H_{84}O_{30}$	$[PFS\text{-}2032+2H]^{2+}$	583.2596	tbd
PFS-2032	$C_{50}H_{84}O_{30}$	$[PFS\text{-}2032+2Na]^{2+}$	605.2416	352.01
PFS-2062	$C_{100}H_{166}O_{61}$	$[PFS\text{-}2062+3H]^{3+}$	782.3380	tbd
PFS-2062	$C_{100}H_{166}O_{61}$	$[PFS\text{-}2062+3Na]^{3+}$	804.3199	519.29
PFS-2052	$C_{80}H_{132}O_{50}$	$[PFS\text{-}2052+2H]^{2+}$	947.3966	441.21
PFS-2052	$C_{80}H_{132}O_{50}$	$[PFS\text{-}2052+2Na]^{2+}$	969.3785	438.21
PFS-2032	$C_{50}H_{84}O_{30}$	$[PFS\text{-}2032+H]^{+}$	1165.5120	tbd
PFS-2062	$C_{100}H_{166}O_{61}$	$[PFS\text{-}2062+2H]^{2+}$	1173.0034	487.62
PFS-2032	$C_{50}H_{84}O_{30}$	$[PFS\text{-}2032+Na]^{+}$	1187.4940	317.49
PFS-2062	$C_{100}H_{166}O_{61}$	$[PFS\text{-}2062+2Na]^{2+}$	1194.9853	494.78
PFS-3062	$C_{220}H_{358}O_{133}$	$[PFS\text{-}3062+4H]^{4+}$	1283.5402	827.59
PFS-3062	$C_{220}H_{358}O_{133}$	$[PFS\text{-}3062+4Na]^{4+}$	1305.5221	tbd
PFS-3052	$C_{180}H_{292}O_{110}$	$[PFS\text{-}3052+3H]^{3+}$	1406.2513	tbd
PFS-4042	$C_{305}H_{492}O_{184}$	$[PFS\text{-}4042+5H]^{5+}$	1421.3921	1169.53
PFS-3052	$C_{180}H_{292}O_{110}$	$[PFS\text{-}3052+3Na]^{3+}$	1428.2333	703.57
PFS-3062	$C_{220}H_{358}O_{133}$	$[PFS\text{-}3062+3H]^{3+}$	1711.0512	786.06
PFS-3062	$C_{220}H_{358}O_{133}$	$[PFS\text{-}3062+3Na]^{3+}$	1733.0331	790.95
PFS-4052	$C_{380}H_{612}O_{230}$	$[PFS\text{-}4052+5H]^{5+}$	1773.1344	tbd
PFS-4042	$C_{305}H_{492}O_{184}$	$[PFS\text{-}4042+4H]^{4+}$	1776.4883	960.68
PFS-4062	$C_{460}H_{742}O_{277}$	$[PFS\text{-}4062+6H]^{6+}$	1785.0767	tbd
PFS-4052	$C_{380}H_{612}O_{230}$	$[PFS\text{-}4052+5Na]^{5+}$	1795.1163	tbd
PFS-4042	$C_{305}H_{492}O_{184}$	$[PFS\text{-}4042+4Na]^{4+}$	1798.4702	975.23
PFS-4062	$C_{460}H_{742}O_{277}$	$[PFS\text{-}4062+6Na]^{6+}$	1807.0587	tbd
PFS-2052	$C_{80}H_{132}O_{50}$	$[PFS\text{-}2052+H]^{+}$	1893.7859	tbd
PFS-2052	$C_{80}H_{132}O_{50}$	$[PFS\text{-}2052+Na]^{+}$	1915.7679	411.72
PFS-3052	$C_{180}H_{292}O_{110}$	$[PFS\text{-}3052+2H]^{2+}$	2108.8733	tbd
PFS-3052	$C_{180}H_{292}O_{110}$	$[PFS\text{-}3052+2Na]^{2+}$	2130.8553	676.89
PFS-4062	$C_{460}H_{742}O_{277}$	$[PFS\text{-}4062+5H]^{5+}$	2141.8906	1232.77
PFS-4062	$C_{460}H_{742}O_{277}$	$[PFS\text{-}4062+5Na]^{5+}$	2163.8726	1097.46
PFS-4052	$C_{380}H_{612}O_{230}$	$[PFS\text{-}4052+4H]^{4+}$	2216.1661	1084.99
PFS-4052	$C_{380}H_{612}O_{230}$	$[PFS\text{-}4052+4Na]^{4+}$	2238.1481	1091.96
PFS-4042	$C_{305}H_{492}O_{184}$	$[PFS\text{-}4042+3H]^{3+}$	2368.3153	tbd
PFS-4042	$C_{305}H_{492}O_{184}$	$[PFS\text{-}4042+3Na]^{3+}$	2390.2972	947.71
PFS-5042	$C_{625}H_{1004}O_{376}$	$[PFS\text{-}5042+6H]^{6+}$	2423.3356	1494.25
PFS-5042	$C_{625}H_{1004}O_{376}$	$[PFS\text{-}5042+6Na]^{6+}$	2445.3175	tbd
PFS-3062	$C_{220}H_{358}O_{133}$	$[PFS\text{-}3062+2H]^{2+}$	2566.0731	tbd
PFS-3062	$C_{220}H_{358}O_{133}$	$[PFS\text{-}3062+2Na]^{2+}$	2588.0550	760.57
PFS-5052	$C_{780}H_{1252}O_{470}$	$[PFS\text{-}5052+7H]^{7+}$	2593.7843	tbd
PFS-5052	$C_{780}H_{1252}O_{470}$	$[PFS\text{-}5052+7Na]^{7+}$	2615.7662	tbd
PFS-4062	$C_{460}H_{742}O_{277}$	$[PFS\text{-}4062+4H]^{4+}$	2677.1115	tbd
PFS-4062	$C_{460}H_{742}O_{277}$	$[PFS\text{-}4062+4Na]^{4+}$	2699.0934	1213.38

PFS-5042	$C_{625}H_{1004}O_{376}$	[PFS-5042+5H]$^{5+}$	2907.8013	tbd
PFS-5042	$C_{625}H_{1004}O_{376}$	[PFS-5042+5Na]$^{5+}$	2929.7832	tbd
PFS-4052	$C_{380}H_{612}O_{230}$	[PFS-4052+3H]$^{3+}$	2954.5524	tbd
PFS-4052	$C_{380}H_{612}O_{230}$	[PFS-4052+3Na]$^{3+}$	2976.5343	tbd
PFS-5052	$C_{780}H_{1252}O_{470}$	[PFS-5052+6H]$^{6+}$	3025.9138	1679.77
PFS-5052	$C_{780}H_{1252}O_{470}$	[PFS-5052+6Na]$^{6+}$	3047.8957	tbd
PFS-5052	$C_{780}H_{1252}O_{470}$	[PFS-5052+5H]$^{5+}$	3630.8951	tbd
PFS-5042	$C_{625}H_{1004}O_{376}$	[PFS-5042+4H]$^{4+}$	3634.4998	tbd
PFS-5052	$C_{780}H_{1252}O_{470}$	[PFS-5052+5Na]$^{5+}$	3652.8770	tbd
PFS-5042	$C_{625}H_{1004}O_{376}$	[PFS-5042+4Na]$^{4+}$	3656.4817	tbd

Emily R. Sekera, Árpád Somogyi, Zoltan Takáts, Florian Stappert, Cedric Thom, Oliver J. Schmitz, Claudia Moeckel, Béla Paizs, Jens Sommertune: Utilization of bis-MPA Dendrimers for the Calibration of Ion Mobility Collision Cross Section Calculations; J. Am. Soc. Mass Spectrom. 2024, 35, 6, 1101–1109

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.

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

Component ID	Chemical Formula	*Ion*	*m/z*	$^{DT}CCS_{N2}$
PFS-2032	$C_{50}H_{84}O_{30}$	[PFS-2032-2H]$^{2-}$	581.244	tbd
PFS-2032	$C_{50}H_{84}O_{30}$	[PFS-2032-2(FA-H)]$^{2-}$	627.249	tbd
PFS-2032	$C_{50}H_{84}O_{30}$	[PFS-2032-2(TFA-H)]$^{2-}$	695.237	tbd
PFS-2062	$C_{100}H_{166}O_{61}$	[PFS-2062-3H]$^{3-}$	780.322	tbd
PFS-2062	$C_{100}H_{166}O_{61}$	[PFS-2062-3(FA-H)]$^{3-}$	826.328	tbd
PFS-2062	$C_{100}H_{166}O_{61}$	[PFS-2062-3(TFA-H)]$^{3-}$	894.315	tbd
PFS-2052	$C_{80}H_{132}O_{50}$	[PFS-2052-2H]$^{2-}$	945.381	tbd
PFS-2052	$C_{80}H_{132}O_{50}$	[PFS-2052-2(FA-H)]$^{2-}$	991.386	tbd
PFS-2052	$C_{80}H_{132}O_{50}$	[PFS-2052-2(TFA-H)]$^{2-}$	1059.374	tbd
PFS-2032	$C_{50}H_{84}O_{30}$	[PFS-2032-H]$^{-}$	1163.496	tbd
PFS-2062	$C_{100}H_{166}O_{61}$	[PFS-2062-2H]$^{2-}$	1170.988	tbd
PFS-2032	$C_{50}H_{84}O_{30}$	[PFS-2032-(FA-H)]$^{-}$	1209.502	tbd
PFS-2062	$C_{100}H_{166}O_{61}$	[PFS-2062-2(FA-H)]$^{2-}$	1216.993	tbd
PFS-2032	$C_{50}H_{84}O_{30}$	[PFS-2032-(TFA-H)]$^{-}$	1277.489	tbd
PFS-3062	$C_{220}H_{358}O_{133}$	[PFS-3062-4H]$^{4-}$	1281.525	tbd
PFS-2062	$C_{100}H_{166}O_{61}$	[PFS-2062-2(TFA-H)]$^{2-}$	1284.981	tbd
PFS-3062	$C_{220}H_{358}O_{133}$	[PFS-3062-4(FA-H)]$^{4-}$	1327.530	tbd
PFS-3062	$C_{220}H_{358}O_{133}$	[PFS-3062-4(TFA-H)]$^{4-}$	1395.517	tbd
PFS-3052	$C_{180}H_{292}O_{110}$	[PFS-3052-3H]$^{3-}$	1404.236	tbd
PFS-3052	$C_{180}H_{292}O_{110}$	[PFS-3052-3(FA-H)]$^{3-}$	1450.241	tbd

PFS-3052	$C_{180}H_{292}O_{110}$	[PFS-3052-3(TFA-H)]$^{3-}$	1518.229	tbd
PFS-3062	$C_{220}H_{358}O_{133}$	[PFS-3062-3H]$^{3-}$	1709.036	tbd
PFS-3062	$C_{220}H_{358}O_{133}$	[PFS-3062-3(FA-H)]$^{3-}$	1755.041	tbd
PFS-4052	$C_{380}H_{612}O_{230}$	[PFS-4052-5H]$^{5-}$	1771.119	tbd
PFS-4062	$C_{460}H_{742}O_{277}$	[PFS-4062-6H]$^{6-}$	1783.061	tbd
PFS-4042	$C_{305}H_{492}O_{184}$	[PFS-4042-4H]$^{4-}$	1798.470	tbd
PFS-4052	$C_{380}H_{612}O_{230}$	[PFS-4052-5(FA-H)]$^{5-}$	1817.124	tbd
PFS-4042	$C_{305}H_{492}O_{184}$	[PFS-4042-4(FA-H)]$^{4-}$	1820.478	tbd
PFS-3062	$C_{220}H_{358}O_{133}$	[PFS-3062-3(TFA-H)]$^{3-}$	1823.028	tbd
PFS-4062	$C_{460}H_{742}O_{277}$	[PFS-4062-6(FA-H)]$^{6-}$	1829.067	tbd
PFS-4052	$C_{380}H_{612}O_{230}$	[PFS-4052-5(TFA-H)]$^{5-}$	1885.112	tbd
PFS-4042	$C_{305}H_{492}O_{184}$	[PFS-4042-4(TFA-H)]$^{4-}$	1888.466	tbd
PFS-2052	$C_{80}H_{132}O_{50}$	[PFS-2052-H]$^{-}$	1891.770	tbd
PFS-4062	$C_{460}H_{742}O_{277}$	[PFS-4062-6(TFA-H)]$^{6-}$	1897.054	tbd
PFS-2052	$C_{80}H_{132}O_{50}$	[PFS-2052-(FA-H)]$^{-}$	1937.776	tbd
PFS-2052	$C_{80}H_{132}O_{50}$	[PFS-2052-(TFA-H)]$^{-}$	2005.763	tbd
PFS-3052	$C_{180}H_{292}O_{110}$	[PFS-3052-2H]$^{2-}$	2106.858	tbd
PFS-4062	$C_{460}H_{742}O_{277}$	[PFS-4062-5H]$^{5-}$	2139.875	tbd
PFS-3052	$C_{180}H_{292}O_{110}$	[PFS-3052-2(FA-H)]$^{2-}$	2152.863	tbd
PFS-4062	$C_{460}H_{742}O_{277}$	[PFS-4062-5(FA-H)]$^{5-}$	2185.880	tbd
PFS-4052	$C_{380}H_{612}O_{230}$	[PFS-4052-4H]$^{4-}$	2214.150	tbd
PFS-3052	$C_{180}H_{292}O_{110}$	[PFS-3052-2(TFA-H)]$^{2-}$	2220.851	tbd
PFS-4062	$C_{460}H_{742}O_{277}$	[PFS-4062-5(TFA-H)]$^{5-}$	2253.868	tbd
PFS-4052	$C_{380}H_{612}O_{230}$	[PFS-4052-4(FA-H)]$^{4-}$	2260.156	tbd
PFS-4052	$C_{380}H_{612}O_{230}$	[PFS-4052-4(TFA-H)]$^{4-}$	2328.143	tbd
PFS-4042	$C_{305}H_{492}O_{184}$	[PFS-4042-3H]$^{3-}$	2390.297	tbd
PFS-4042	$C_{305}H_{492}O_{184}$	[PFS-4042-3(FA-H)]$^{3-}$	2412.305	tbd
PFS-5042	$C_{625}H_{1004}O_{376}$	[PFS-5042-6H]$^{6-}$	2421.320	tbd
PFS-5042	$C_{625}H_{1004}O_{376}$	[PFS-5042-6(FA-H)]$^{6-}$	2467.325	tbd
PFS-4042	$C_{305}H_{492}O_{184}$	[PFS-4042-3(TFA-H)]$^{3-}$	2480.293	tbd
PFS-5042	$C_{625}H_{1004}O_{376}$	[PFS-5042-6(TFA-H)]$^{6-}$	2535.313	tbd
PFS-3062	$C_{220}H_{358}O_{133}$	[PFS-3062-2H]$^{2-}$	2564.057	tbd
PFS-5052	$C_{780}H_{1252}O_{470}$	[PFS-5052-7H]$^{7-}$	2591.769	tbd
PFS-3062	$C_{220}H_{358}O_{133}$	[PFS-3062-2(FA-H)]$^{2-}$	2610.063	tbd
PFS-5052	$C_{780}H_{1252}O_{470}$	[PFS-5052-7(FA-H)]$^{7-}$	2637.774	tbd
PFS-4062	$C_{460}H_{742}O_{277}$	[PFS-4062-4H]$^{4-}$	2675.096	tbd
PFS-3062	$C_{220}H_{358}O_{133}$	[PFS-3062-2(TFA-H)]$^{2-}$	2678.050	tbd
PFS-5052	$C_{780}H_{1252}O_{470}$	[PFS-5052-7(TFA-H)]$^{7-}$	2705.761	tbd
PFS-4062	$C_{460}H_{742}O_{277}$	[PFS-4062-4(FA-H)]$^{4-}$	2721.101	tbd
PFS-4062	$C_{460}H_{742}O_{277}$	[PFS-4062-4(TFA-H)]$^{4-}$	2789.089	tbd
PFS-5042	$C_{625}H_{1004}O_{376}$	[PFS-5042-5H]$^{5-}$	2905.786	tbd
PFS-5042	$C_{625}H_{1004}O_{376}$	[PFS-5042-5(FA-H)]$^{5-}$	2951.791	tbd
PFS-4052	$C_{380}H_{612}O_{230}$	[PFS-4052-3H]$^{3-}$	2952.537	tbd
PFS-4052	$C_{380}H_{612}O_{230}$	[PFS-4052-3(FA-H)]$^{3-}$	2998.542	tbd
PFS-5042	$C_{625}H_{1004}O_{376}$	[PFS-5042-5(TFA-H)]$^{5-}$	3019.778	tbd

PFS-5052	$C_{780}H_{1252}O_{470}$	[PFS-5052-6H]$^{6-}$	3023.898	tbd
PFS-4052	$C_{380}H_{612}O_{230}$	[PFS-4052-3(TFA-H)]$^{3-}$	3066.530	tbd
PFS-5052	$C_{780}H_{1252}O_{470}$	[PFS-5052-6(FA-H)]$^{6-}$	3069.904	tbd
PFS-5052	$C_{780}H_{1252}O_{470}$	[PFS-5052-6(TFA-H)]$^{6-}$	3137.891	tbd
PFS-5052	$C_{780}H_{1252}O_{470}$	[PFS-5052-5H]$^{5-}$	3628.879	tbd
PFS-5042	$C_{625}H_{1004}O_{376}$	[PFS-5042-4H]$^{4-}$	3632.484	tbd
PFS-5052	$C_{780}H_{1252}O_{470}$	[PFS-5052-5(FA-H)]$^{5-}$	3674.885	tbd
PFS-5042	$C_{625}H_{1004}O_{376}$	[PFS-5042-4(FA-H)]$^{4-}$	3678.490	tbd
PFS-5052	$C_{780}H_{1252}O_{470}$	[PFS-5052-5(TFA-H)]$^{5-}$	3742.872	tbd
PFS-5042	$C_{625}H_{1004}O_{376}$	[PFS-5042-4(TFA-H)]$^{4-}$	3746.477	tbd

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.