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Product Information

MS QCAL Peptide Mix

Catalog Number **MSQC2**
Storage Temperature 2-8 °C

Product Description

Protein and peptide standards are critical in mass spectrometry (MS)-based proteomics to ensure both quality sample preparation as well as optimal system performance. Peptide standards may be used to confirm that chromatography, peptide elution, and MS systems are working properly.[1]

This product (MSQC2) is a mixture of 22 peptides derived from the trypsin digested protein concatamer QCAL.[2] QCAL was designed using the QconCAT technology,[3] recombinantly expressed in *E. coli,* purified, and quantitated with amino acid analysis. The parent protein sequence of QCAL is as follows:

MGALRVFDEFKPLVEEPQNLIRVFDEFKPLVKPEEPQ
NLIRVFDEFKPLVKPEEKPQNLIRVFDEFKPLVKPEEK
PQNKPLIRVFKPDEFKPLVKPEEKPQNKPLIRVFKPDE
FKPLVKPEEKPQNKPLIKPRVFDEFQPLVEEPQNLIRG
VNDNEEGFFSARGGVNDNEEGFFSARGGVNDNEEG
FFSARGGVNDNEEGFFSARGGGVNDNEEGFFSARG
GGVNDNEEGFFSARGGGVNDNEEGFFSARGGGVN
DNEEGFFSARGGGVNDNEEGFFSARGVNDNEEGFF
SAKGGGVNDNEEGFFSARAVMDDFAAFVEKAVMMD
DFAAFVEKAVMMMDDFAAFVEKGLVKFVVPRALELF
RIGDYAGIKEALDFFARYLGYLEQLLRVLYPNDNFFEG
KLFTFHADICTLPDTEKALVALVLVPRGSLEVLFQGPIE
GRTENLYFQGDDDDKALVALVHHHHHH

QCAL was then digested with trypsin, to give the product MSQC2. The masses of the QCAL peptides range from 415–3,100 Da.

MSQC2 is intended to act as a universal MS platform standard, by providing several elements for calibration and performance assessment. These elements include:

- Instrument resolution: peptides 20 and 21 of MSQC2 are identical, except for a Lys→Glu substitution, to provide a pair of peptides whose masses differ by 0.0364 Da. Discriminating these two peptides requires an instrument resolution of ≥57,000 (FWHM). Thus differentiation of these peptides can be used as a benchmark for instrument resolution.
- Linearity of signal detection: peptides 11, 14, and 16 differ only by the number of glycine residues at their amino termini (one, two, and three, respectively). As well, MSQC2 contains one copy of peptide 11, three copies of peptide 14, and six copies of peptide 16. Thus these peptides can serve as a benchmark for signal linearity on an LC-MS instrument.

Table 1, List of Peptides and Molecular Masses, includes 5 peptides that are derived from the poly-histidine tag, which is used for affinity purification of the protein, and from the linker sequence. These peptides (6, 9, 15, 17, and 26) are not part of the intended product performance features of QCAL. However, because these peptides do give peaks in LC analysis, they are listed for clarity.

Components

MS QCAL Peptide Mix 2 × 25 μg vials
Catalog Number MSQC2
Each vial contains 25 μg of lyophilized peptides.

Storage/Stability

Storage of this product at 2-8 °C is recommended.

Precautions and Disclaimer

This product is for R&D use only, not for drug, household, or other uses. Please consult the Safety Data Sheet for information regarding hazards and safe handling practices.

Preparation Instructions

MSQC2 is soluble in reagents that are compatible with proteomics workflows (e.g., 0.1% formic acid/water, 0.1% trifluoroacetic acid/water).

Centrifuge the vial at ~10,000 × *g* to collect the product at the bottom. Upon addition of liquid to the vial, vortex rigorously. Aliquot the reconstituted MSQC2 peptide solution and store frozen at -70 °C for up to 6 months.

After solubilization in an appropriate buffer, MSQC2 can be directly injected for LC-MS analysis.

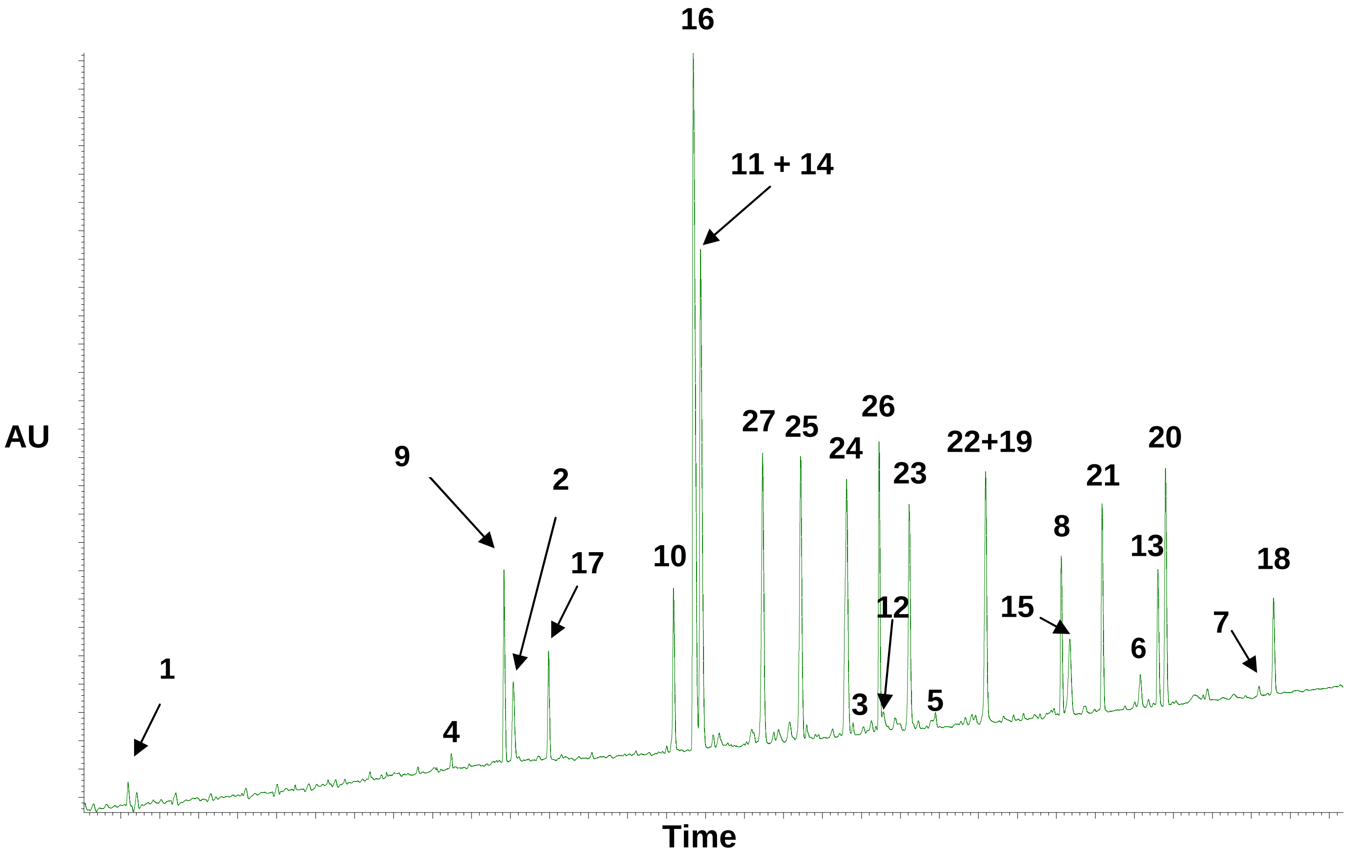
The final product is lyophilized from a 0.1 mg/mL solution containing 2,2,2-trifluoroethanol (TFE), bis-tris propane, Tris(2-carboxyethyl)phosphine (TCEP), and iodoacetamide, as well as some residual active trypsin. Upon reconstitution, some digestion buffer components will be present in the sample. As an example, if the sample is reconstituted in 100 μL, the amount of residual buffer components remaining will be about 20 mM bis-tris propane, 0.3 mM TCEP, and 0.3 mM iodoacetamide.

References

1. Nilsson, T. *et al.*, Mass spectrometry in high-throughput proteomics: ready for the big time. *Nat. Methods*, **7(9)**, 681-685 (2010).
2. Eyers, C.E. *et al.*, QCAL - A novel standard for assessing instrument conditions for proteome analysis. *J. Am. Soc. Mass Spectrom.*, **19(9)**, 1275-1280 (2008).
3. Pratt, J.M. *et al.*, Multiplexed absolute quantification for proteomics using concatenated signature peptides encoded by QconCAT genes. *Nat. Protoc.*, **1(2)**, 1029-1043 (2006).

GCY,JJW,KR,KV,MAM 01/17-1

Figure 1.
Representative UV Chromatogram of MSQCAL Digest



Instrumentation:

- HPLC- Waters ACQUITY UPLC® with PDA Detector with two Ascentis® Express Peptide ES-C_{18} Columns Connected in Series
- MS- Waters Q-TOF Premier™ Mass Spectrometer

Table 1.
List of Peptides and Molecular Masses

Peptide #	Sequence	Calibration Element	$[M+H]^+$	$[M+2H]^{2+}$	$[M+3H]^{3+}$
1	GLVK	m/z	416.2872	208.6475	139.4343
2	FVVPR	m/z, LC	617.3775	309.1926	206.4644
3	ALELFR	m/z, LC	748.4357	374.7217	250.1504
4	IGDYAGIK	m/z, LC	836.4517	418.7298	279.4891
5	EALDFFAR	m/z, LC	968.4841	484.7459	323.4999
6 (*)	ALVALVLVPR	Expression System	1050.7039	525.8558	350.9065
7	YLGYLEQLLR	m/z, LC	1267.7050	634.3564	423.2402
8	AVMDDFAAFVEK	m/z, LC, Met Ox	1342.6352	671.8215	448.2169
9 (*)	ALVALVHHHHHH	Expression System	1407.751	704.3794	469.9222
10	GVNDNEEGFFSAK	guanidation	1413.6286	707.3182	471.8814
11	GVNDNEEGFFSAR	Linearity of response	1441.6347	721.3213	481.2168
12	VLYPNDNFFEGK	m/z, LC	1442.6955	721.8517	481.5704
13	AVMMDDFAAFVEK	m/z, LC, Met Ox	1473.6757	737.3418	491.8971
14	GGVNDNEEGFFSAR	Linearity of response	1498.6562	749.8320	500.2239
15 (*)	GSLEVLFQGPIEGR	Expression System	1501.8014	751.4046	501.2723
16	GGGVNDNEEGFFSAR	Linearity of response	1555.6777	778.3427	519.2311
17 (*)	TENLYFQGDDDDK	Expression System	1559.6501	780.3289	520.5552
18	AVMMMDDFAAFVEK	m/z, LC, Met Ox	1604.7162	802.8620	535.5772
19	LFTFHADI(Cam)TLPDTEK (Cam: alkylation with iodoacetamide)	m/z, LC	1907.9213	954.4645	636.6456
20	VFDEFQPLVEEPQNLIR	m/z, resolution, LC	2073.0656	1037.0367	691.6937
21	VFDEFKPLVEEPQNLIR	m/z, resolution, LC	2073.1020	1037.0549	691.7059
22	VFDEFKPLVKPEEPQNLIR	m/z, resolution, LC	2298.2497	1149.6288	766.7551
23	VFDEFKPLVKPEEKPQNLIR	m/z, resolution, LC	2426.3447	1213.6762	809.4534
24	VFDEFKPLVKPEEKPQNKPLIR	m/z, resolution, LC	2651.4924	1326.2501	884.5027
25	VFKPDEFKPLVKPEEKPQNKPLIR	m/z, resolution, LC	2876.6401	1438.8240	959.5519
26 (*)	TENLYFQGDDDDKALVALVHHHHHH	Expression System	2948.3827	1474.6953	983.4661
27	VFKPDEFKPLVKPEEKPQNKPLIKPR	m/z, resolution, LC	3101.7878	1551.3978	1034.6011

(*) Peptides 6, 9, 15, 17, and 26 are derived from the poly-histidine tag which is used for affinity purification of the protein, and from the linker sequence. These peptides are not part of the intended product performance features of QCAL. However, because these peptides do give peaks in LC analysis, they are listed here for clarity.