Electronic Supplementary Material (ESI) for ChemComm.

Identification of actin as a direct proteomic target of berberine, using an affinity-based chemical probe and elucidation of its modulatory role in actin assembly

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Experimental section

Chemistry

General methods. Unless otherwise described, all commercial reagents and solvents were purchased from commercial suppliers such as Sigma-Aldrich, and used without further purifications. Tetrahydrofuran was distilled from sodium benzophenone ketyl and dichloromethane, acetonitrile, triethylamine and pyridine were freshly distilled with calcium hydride. Flash column chromatography was carried out using silica-gel 60 (230-400 mesh, Merck). Thin layer chromatography was performed using 0.25 mm silica gel plates to monitor reactions. All reactions were performed under dry argon atmosphere in flame-dried glassware. ^{1}H NMR and ^{13}C NMR spectra were recorded on a BRUKER AVANCE 400 (400MHz), or VARIAN VNMRS 500 (500MHz) spectrometers, respectively. Chemical shifts are provided in parts per million (ppm, δ) downfield from tetramethylsilane (internal standard) with coupling constant in hertz (Hz). Multiplicity is indicated by the following abbreviations: singlet (s), doublet (d), doublet of doublet (dd), triplet (t), quartet (q), quintet (quin) multiplet (m) and broad (br). Optical rotations were measured using JASCO DIP-1000 digital polarimeter at ambient temperature using 100 nm cell of 2 mL capacity. Mass spectra and HRMS were recorded on Agilent 6530 Accurate-Mass Q-TOF LC/MS and JEOL JMS-700. The purity of the compounds was identified by normal phase high-pressure liquid chromatography (HPLC) is carried out either on.

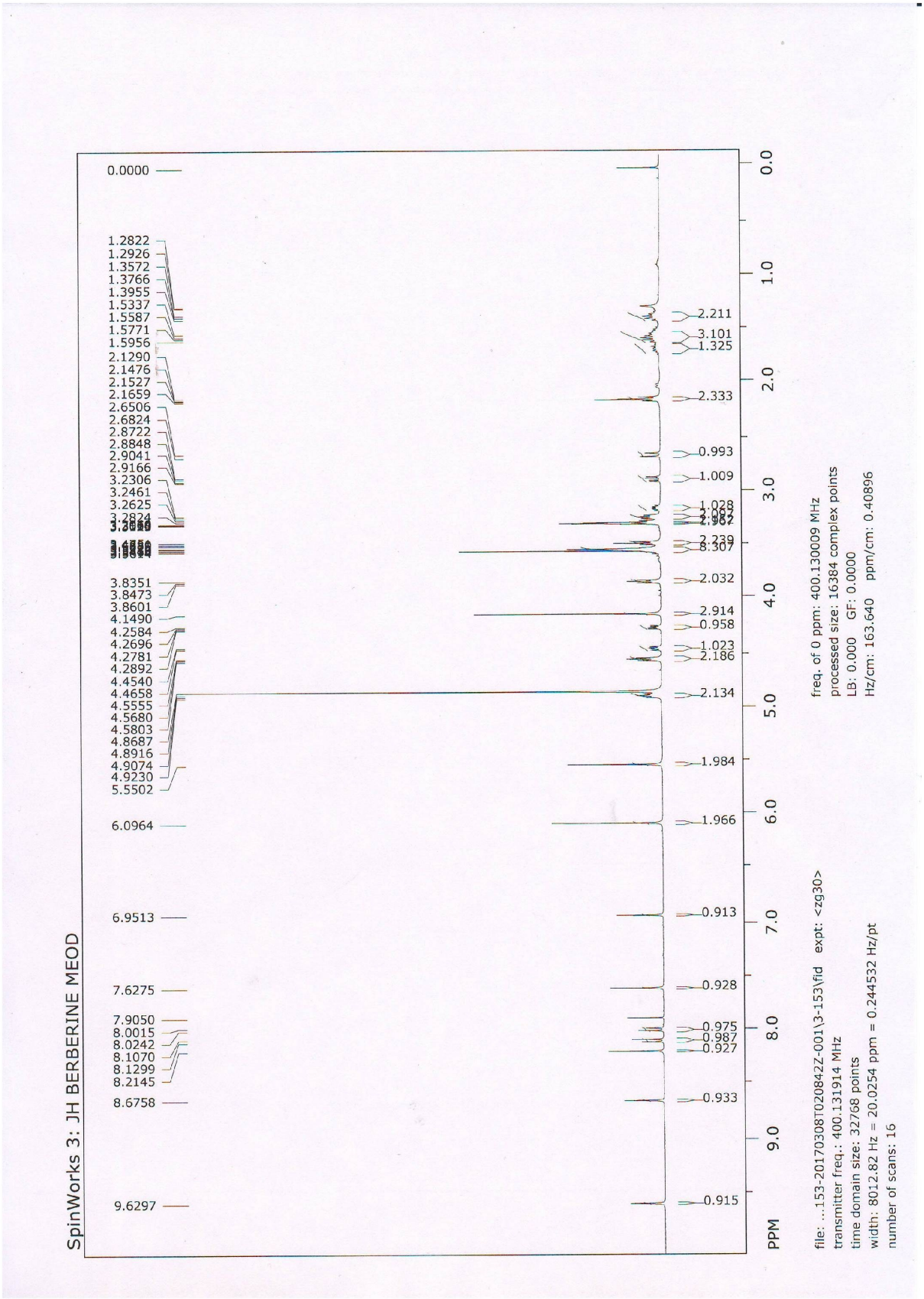
Compound (2) To a solution of **1** (1.006 mmol, ref: *Anticancer Agents Med. Chem.,* **2015**, *15*, 89-98.) in DMF (10 mL) was added propargyl bromide (2.415 mmol). The reaction mixture was stirred at 80 °C until complete consumption of the starting material on TLC. The reaction mixture was recrystallized from diethyl ether to afford 398mg (100%) of compound **2** as a brown solid. ^{1}H-NMR (DMSO, 300 MHz) δ 9.88 (s, 1H), 8.97 (d, 1H, *J* = 7.8 Hz), 8.22 (t, 1H, *J* = 8.8 Hz), 8.03 (dd, 1H, *J* = 14.8, 9.1 Hz), 7.80 (s, 1H), 7.09 (s, 1H), 6.18 (s, 2H), 5.09 (d, 2H, *J* = 2.4 Hz), 4.96 (t, 2H, *J* = 6.1 Hz), 4.09 (d, 3H, *J* = 5.6 Hz), 3.62 (t, 1H, *J* = 2.4 Hz), 3.21 (t, 2H, *J* = 6.1 Hz); ^{13}C-NMR (DMSO, 75 MHz) δ 151.2, 150.4, 148.2, 145.8, 141.2, 138.1, 133.4, 131.2, 127.0, 124.8, 122.6, 120.9, 120.8, 108.9, 106.0, 102.6, 80.3, 79.3, 61.4, 57.7, 55.8, 26.8; LR-MS (FAB) *m/z* 360 $(M\text{-}Cl)^{+}$; HR-MS (FAB) calculated for $C_{22}H_{18}NO_4^{+}$ $(M\text{-}Cl)^{+}$ 360.1236; found 360.1237.

Compound (4) To a solution of **2** (0.253 mmol), and *N*-[2-[2-[2-(2-azidoethoxy)ethoxy]-ethoxy]ethyl]-biotinamide (**3**, 0.253 mmol) in *t*-BuOH (3 mL) and H_2O (3 mL) were added sodium ascorbate (0.487 mmol) and copper(II) sulfate (0.152 mmol). The reaction mixture was stirred at room temperature until complete consumption of the starting material on TLC. Then, the solvent was concentrated *in vacuo* and purified by column chromatography on silica gel (methylene chloride:

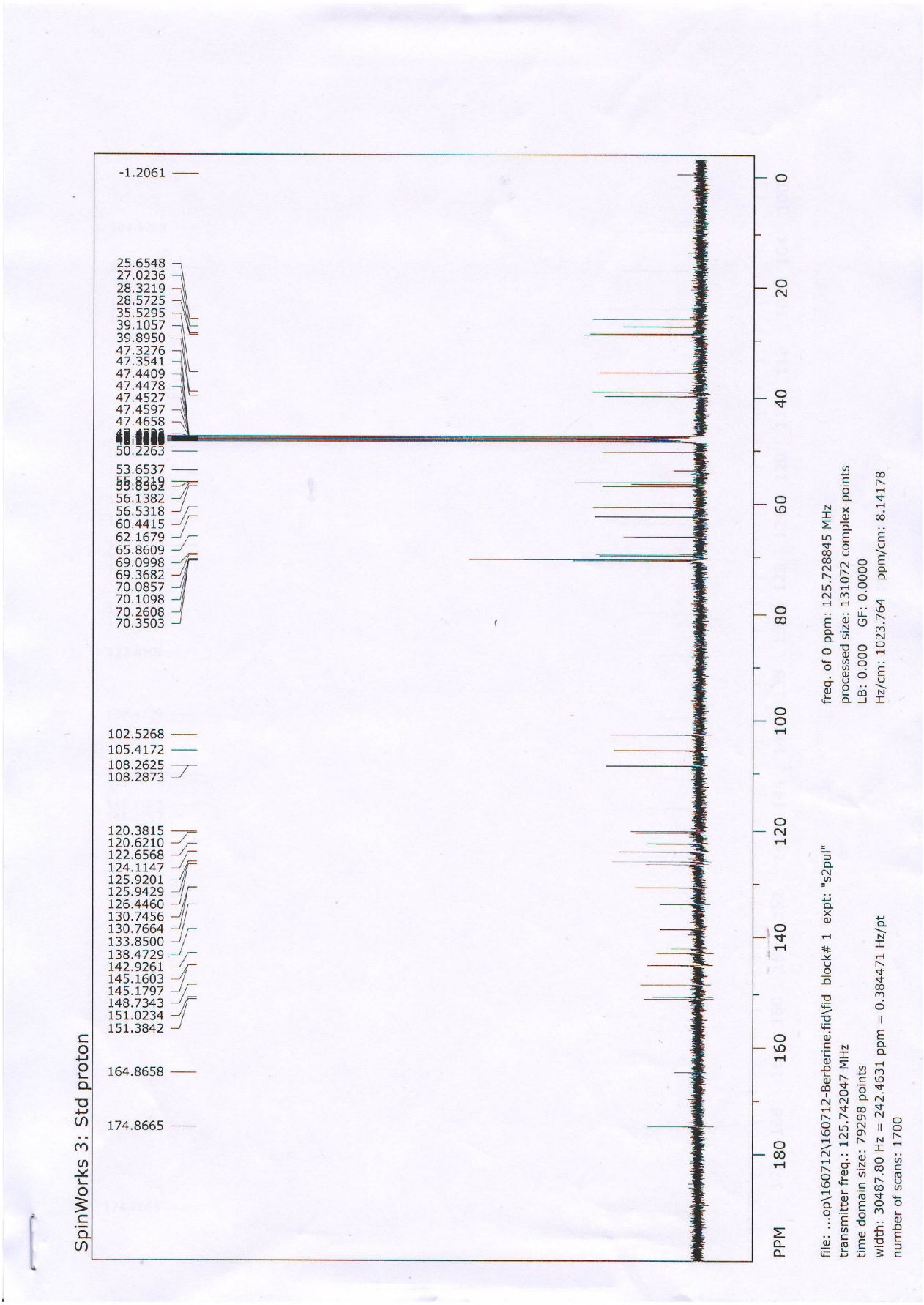
methanol: water = 70:14:1) to afford 60 mg (28%) of compound **3** as a yellow solid; ^{1}H-NMR (MeOD, 400 MHz) δ 9.63 (s, 1H), 8.68 (s, 1H), 8.21 (s, 1H), 8.12 (d, 1H, *J* = 9.2 Hz), 8.01 (d, 1H, *J* = 9.1 Hz), 7.63 (s, 1H), 6.95 (s, 1H), 6.10 (s, 2H), 5.55 (s, 2H), 4.91 (t, 2H, *J* = 6.3 Hz), 4.57 (t, 2H, *J* = 5.0 Hz), 4.47 (dd, 1H, *J* = 7.8, 4.8 Hz), 4.27 (dd, 1H, *J* = 7.9, 4.5 Hz), 4.15 (s, 3H), 3.85 (t, 2H, *J* = 5.0 Hz), 3.56-3.53 (m, 8H), 3.49 (t, 2H, *J* = 5.7 Hz), 3.31-3.29 (m, 2H), 3.25 (t, 2H, *J* = 6.6 Hz), 3.19-3.14 (m, 1H), 2.89 (m, 1H), 2.67 (d, 1H, *J* = 12.7 Hz), 2.17-2.13 (m, 2H), 1.67-1.29 (m, 6H); ^{13}C-NMR (MeOD, 125 MHz) δ 174.9, 164.9, 151.4, 151.0, 148.7, 145.2, 142.3, 142.1, 138.5, 133.9, 130.8, 126.4, 125.9, 124.1, 122.7, 120.6, 120.4, 108.3, 105.4, 102.5, 70.4, 70.3, 70.1, 69.4, 69.1, 65.9, 62.2, 60.4, 56.5, 56.1, 55.8, 53.7, 50.2, 39.9, 39.1, 35.5, 28.6, 28.3, 27.0, 25.7; LR-MS (ESI) *m/z* 804 $(M\text{-}Cl)^{+}$; HR-MS (ESI) calculated for $C_{40}H_{50}N_7O_9S^{+}$ $(M\text{-}Cl)^{+}$ 804.3385; found 804.3377.

Compound 4 (BBP)

▼ ^{1}H-NMR ($CDCl_3$, 400 MHz)



▼ ^{13}C-NMR ($CDCl_3$, 125 MHz)



Biological assay

Pull-down assay

Jurkat human leukemic T-cells (ATCC TIB-152) were maintained in RPMI medium containing 10% FBS and penicillin/streptomycin (100 U/ml). Jurkat cells were lysed with lysis buffer (XX mM Tris-HCl containing 0.25% NP-40 and protease inhibitor cocktail). The lysates (10 mg) were incubated with Biotin-azide (20 μM) or Berberine biotinylated probe (BBP) (20 μM) with or without free berberine (40 μM) for 2 hours, followed by further incubation with streptavidin-resin for 30 minutes. After extensive washing with lysis buffer 5 times, BBP-bound proteins were eluted with SDS-PAGE sample buffer and subjected to SDS-PAGE and silver staining according to the manufacturer's instruction (Pierce). The band was excised and analyzed using LC-MS/MS by Yonsei Proteome Research Center (YPRC).

LC-MS/MS for peptide analysis

NanoLC–MS/MS analysis was performed on an agilent 1100 Series nano-LC and LTQ- mass spectrometer (Thermo Electron, San Jose, CA). The capillary column used for LC–MS/MS analysis (150 mm × 0.075 mm) was obtained from Proxeon (Odense M , Denmark) and slurry packed in house with 5 μm, 100 Å pore size Magic C18 stationary phase (Michrom Bioresources, Auburn, CA). The mobile phase A for the LC separation was 0.1% formic acid in deionized water and the mobile phase B was 0.1% formic acid in acetonitrile. The chromatography gradient was set up to give a linear increase from 6 % B to 50 % B in 17 min and from 50 % B to 95 % B in 6 min and from 95 % B to 6 % B in 12 min. The flow rate was maintained at 600 nL/min after splitting. Mass spectra were acquired using data-dependent acquisition with full mass scan (350-1800 m/z) followed by MS/MS scans. Each MS/MS scan acquired was an average of one microscans on the LTQ. The temperature of the ion transfer tube was controlled at 200 ℃ and the spray was 1.5.0-2.0 kV. The normalized collision energy was set at 35% for MS/MS.

Database searching

The mascot algorithm (Matrixscience, USA) was used to identify peptide sequences present in a protein sequence database. Database search criteria were, taxonomy; *homo sapiens* (NCBInr database downloaded on Mar 24 2013; 695124 sequences: 228548881 residues), fixed modification; carboxyamidomethylated at cysteine residues, variable modification; oxidized at methionine residues, maximum allowed missed cleavage; 2, MS tolerance; 1.2 Da, MS/MS tolerance; 0.6 Da. Only peptides resulting from trypsin digests were considered.

Direct binding assay

Purified rabbit actin (13.5 μg) was reacted with BBP (20 μM) with or without free berberine (BBR, 40 μM) for 2 hours followed by dialysis using Tris-HCl (pH 8.0) buffer to remove free BBP. The samples were further incubated with streptavidin resin for 30 minutes and washed with Tris-HCl buffer five times. Precipitated samples were subjected to SDS-PAGE and silver staining (Pierce) according to the instruction. To further confirm the interaction between berberine and actin Surface Plasmon Resonance (SPR) assay was carried out.

Podosome reformation assay

Raw 264.7 cells (ATCC TIB-71) were maintained in Dulbecco's modified Eagle's medium (DMEM) containing 10% FBS and penicillin/streptomycin (100 U/ml). Cells were starved for 24 hours with serum-free DMEM, then treated with 25 μM PP2 for 30 minutes to remove podosomes. After podosome disruption, cells were washed with phosphate buffered saline (PBS) and fed with normal complete medium containing DMSO or BBR (100 μM). After 30 minutes of incubation, cells were washed once with PBS and then fixed with 4% paraformaldehyde for an hour. Fixed cells were washed with PBS once and permeabilized with 0.1% Triton-X100 for 15 min. After permeabilization, cells were washed two or more times with PBS and stained with CytoPainter F-actin staining kit-Green Fluorescence (Abcam) for an hour to visualize newly formed podosomes.

Actin polymerization and depolymerization Assay

In vitro actin polymerization and depolymerization assays were carried out using fluorescence-based actin polymerization kit (Cytoskeleton, Cat. No. BK003) according to the manufacturer's instruction. Briefly, polymerization buffer (10X) was added to prepared pyrene-G-actin samples with indicated concentrations of free berberine. Actin polymerization was assessed by monitoring fluorescence signal using a fluorimeter (Tecan). To assess the depolymerizing activity of berberine, pyrene F-actin was prepared by polymerization of G-actin for 1 hour according to the instruction. Indicated concentrations of berberine were added to the samples and depolymerization was monitored for 90 minutes using a fluorimeter.

Imaging of actin filaments after the treatment of berberine.

NIH3T3 cell line was cultured in DMEM supplemented with 10% fetal bovine serum (Hyclone), 2 mM L-glutamine, 1 U/ml penicillin, 100 mg/ml streptomycin, and 1 mM sodium pyruvate. For imaging experiment, cells were plated onto 35 mm glass coverslip-bottomed dishes coated with 10 μg/ml of

fibronectin (Invitrogen). Cells were washed once with pre-chilled phosphate buffered saline (PBS) and incubated with PBS containing 25 μl/ml 0.1% Triton-X100 for 10 min at 4°C. Then, the cells were washed once with pre-warmed media and returned to the incubator with culture media with or without 100 μM berberine chloride. After 48 hours of incubation, cells were washed once with pre-warmed PBS and then fixed with 4% paraformaldehyde. Fixed cells were washed two or more times with PBS for 10 min and permeabilized with pre-chilled 0.1%Triton-X100 for 5 min, after washed again and then, blocked with 1% BSA (company) for 30 minutes in room temperature. After blocking, cells were washed two or more times with PBS for 10 minutes and stained with PBS containing Alexa Fluor 594 Phalloidin (1:200)(Life technology) for 30 minutes. Images were collected by a Nikon Ti-E inverted microscope and a cooled charge-coupled device camera using NIS software with a 560DF40 excitation filter, a 595DRLP dichroic mirror, and a 653DF95 emission filter. A neutral-density filter was used to control the intensity of the excitation light. Collected images were analyzed with NIS software.

Query	Observed	Mr(expt)	Mr(calc)	Delta	Miss	Score	Expect	Rank	Peptide
926	519.2214	1036.4281	1036.2683	0.1597	1	32	3	1	K.IKIIAPPER.K
1094	567.1108	1132.2068	1132.1803	0.0264	0	53	0.023	1	R.GYSFTTTAER.E
213	389.4738	1165.3992	1164.4406	0.9585	2	14	2.5e+02	1	K.IKIIAPPERK.Y
1158	590.0047	1177.9946	1177.3683	0.6263	0	53	0.026	1	K.EITALAPSTMK.I + Oxidation (M)
1161	590.2059	1178.3971	1177.3683	1.0287	0	(40)	0.5	1	K.EITALAPSTMK.I + Oxidation (M)
303	400.2251	1197.6531	1198.4173	-0.7641	0	(21)	28	1	R.AVFPSIVGRPR.H
1188	600.4106	1198.8064	1198.4173	0.3891	0	(52)	0.026	1	R.AVFPSIVGRPR.H
1189	600.7466	1199.4784	1198.4173	1.0611	0	61	0.0047	1	R.AVFPSIVGRPR.H
834	474.2572	1419.7495	1418.6982	1.0513	1	17	96	4	K.EITALAPSTMKIK.I + Oxidation (M)
898	506.7520	1517.2340	1516.5679	0.6660	0	64	0.0015	1	K.QEYDESGPSIVHR.K
965	528.0950	1581.2627	1580.8654	0.3974	1	(2)	2.7e+03	6	R.MQKEITALAPSTMK.I + 2 Oxidation (M)
966	528.1721	1581.4942	1580.8654	0.6288	1	44	0.15	1	R.MQKEITALAPSTMK.I + 2 Oxidation (M)
1724	896.2137	1790.4127	1790.9243	-0.5116	0	(58)	0.0048	1	K.SYELPDGQVITIGNER.F
1725	896.2207	1790.4266	1790.9243	-0.4977	0	84	1.1e-05	1	K.SYELPDGQVITIGNER.F
1212	608.3723	1822.0948	1822.1953	-0.1005	2	15	1.4e+02	1	R.MQKEITALAPSTMKIK.I + 2 Oxidation (M)
1759	977.8463	1953.6778	1954.2269	-0.5491	0	41	0.25	2	R.VAPEEHPVLLTEAPLNPK.A
1342	652.7145	1955.1213	1954.2269	0.8943	0	(36)	1.3	1	R.VAPEEHPVLLTEAPLNPK.A
1344	652.7909	1955.3505	1954.2269	1.1236	0	(36)	1.3	1	R.VAPEEHPVLLTEAPLNPK.A
1345	652.7914	1955.3520	1954.2269	1.1250	0	(39)	0.61	1	R.VAPEEHPVLLTEAPLNPK.A
1346	652.7930	1955.3567	1954.2269	1.1298	0	(24)	21	1	R.VAPEEHPVLLTEAPLNPK.A
1531	719.6747	2156.0021	2156.4032	-0.4011	1	55	0.011	1	K.AGFAGDDAPRAVFPSIVGRPR.H
1596	765.9501	2294.8282	2295.5931	-0.7649	1	20	46	2	R.VAPEEHPVLLTEAPLNPKANR.E

Supplementary Figure S1. LC-MS/MS analyses of a tryptic digest of the protein band pulled-down by BBP.

Peptide View

MS/MS Fragmentation of **IKIIAPPER**

Found in **gi|28252** in **NCBInr_human**, unnamed protein product [Homo sapiens]

Match to Query 926: 1036.428090 from(519.221436,2+)

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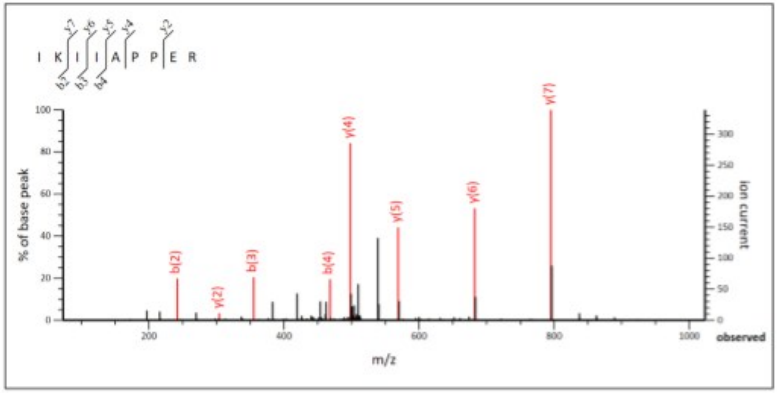

#	b	b^{++}	b*	b^{*++}	b^0	b^{0++}	Seq.	y	y^{++}	y*	y^{*++}	y^0	y^{0++}	#
1	114.1650	57.5862					I							9
2	**242.3373**	121.6723	225.3068	113.1571			K	924.1182	462.5628	907.0877	454.0475	906.1029	453.5551	8
3	**355.4949**	178.2511	338.4644	169.7359			I	***795.9459***	398.4766	778.9154	389.9614	777.9306	389.4690	7
4	**468.6525**	234.8299	451.6220	226.3147			I	***682.7883***	341.8978	665.7578	333.3826	664.7730	332.8902	6
5	539.7304	270.3689	522.6999	261.8536			A	***569.6307***	285.3190	552.6002	276.8038	551.6154	276.3114	5
6	636.8456	318.9265	619.8151	310.4112			P	***498.5528***	249.7801	481.5223	241.2648	480.5375	240.7724	4
7	733.9608	367.4841	716.9303	358.9688			P	401.4376	201.2225	384.4071	192.7072	383.4223	192.2148	3
8	863.0748	432.0411	846.0443	423.5258	845.0595	423.0335	E	***304.3224***	152.6649	287.2919	144.1496	286.3071	143.6572	2
9							R	175.2084	88.1079	158.1779	79.5926			1

Average mass of neutral peptide Mr(calc): 1036.2683 **Fixed modifications:** Carbamidomethyl (C) (apply to specified residues or termini only) **Ions Score:** 32 **Expect:** 3 **Matches :** 8/78 fragment ions using 16 most intense peaks

Peptide View

MS/MS Fragmentation of **GYSFTTTAER**

Found in **gi|28252** in **NCBInr_human**, unnamed protein product [Homo sapiens]

Match to Query 1094: 1132.206776 from(567.110779,2+)

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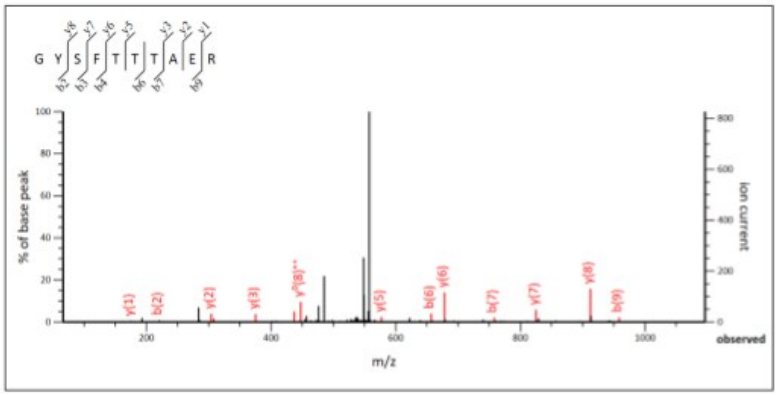

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1	58.0587	29.5330			G							10
2	**221.2320**	111.1197			Y	1076.1365	538.5719	1059.1060	530.0567	1058.1212	529.5643	9
3	**308.3093**	154.6583	290.2940	145.6507	S	***912.9632***	456.9853	895.9327	448.4700	894.9479	447.9776	8
4	455.4832	228.2453	437.4679	219.2377	F	***825.8859***	413.4466	808.8554	404.9314	807.8706	404.4390	7
5	556.5871	278.7972	538.5718	269.7896	T	***678.7120***	339.8597	661.6815	331.3444	660.6967	330.8520	6
6	**657.6910**	329.3492	639.6757	320.3416	T	***577.6081***	289.3077	560.5776	280.7925	559.5928	280.3001	5
7	**758.7949**	379.9011	740.7796	370.8935	T	476.5042	238.7558	459.4737	230.2405	458.4889	229.7481	4
8	829.8728	415.4401	811.8575	406.4325	A	***375.4003***	188.2038	358.3698	179.6886	357.3850	179.1962	3
9	**958.9868**	479.9971	940.9715	470.9895	E	***304.3224***	152.6649	287.2919	144.1496	286.3071	143.6572	2
10					R	***175.2084***	88.1079	158.1779	79.5926			1

Average mass of neutral peptide Mr(calc): 1132.1803 **Fixed modifications:** Carbamidomethyl (C) (apply to specified residues or termini only) **Ions Score:** 53 **Expect:** 0.023 **Matches :** 14/84 fragment ions using 26 most intense peaks

Peptide View

MS/MS Fragmentation of **IKIIAPPERK**

Found in **gi|28252** in **NCBInr_human**, unnamed protein product [Homo sapiens]

Match to Query 213: 1165.399182 from(389.473785,3+)

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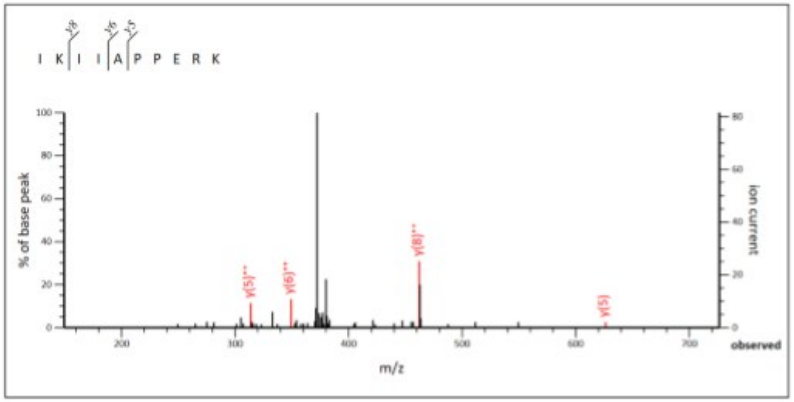

#	b	b^{++}	b^*	b^{*++}	b^0	b^{0++}	Seq.	y	y^{++}	y^*	y^{*++}	y^0	y^{0++}	#
1	114.1650	57.5862					I							10
2	242.3373	121.6723	225.3068	113.1571			K	1052.2905	526.6489	1035.2600	518.1337	1034.2752	517.6413	9
3	355.4949	178.2511	338.4644	169.7359			I	924.1182	***462.5628***	907.0877	454.0475	906.1029	453.5551	8
4	468.6525	234.8299	451.6220	226.3147			I	810.9606	405.9840	793.9301	397.4687	792.9453	396.9763	7
5	539.7304	270.3689	522.6999	261.8536			A	697.8030	***349.4052***	680.7725	340.8899	679.7877	340.3975	6
6	636.8456	318.9265	619.8151	310.4112			P	626.7251	***313.8662***	609.6946	305.3510	608.7098	304.8586	5
7	733.9608	367.4841	716.9303	358.9688			P	529.6099	265.3086	512.5794	256.7934	511.5946	256.3010	4
8	863.0748	432.0411	846.0443	423.5258	845.0595	423.0335	E	432.4947	216.7510	415.4642	208.2358	414.4794	207.7434	3
9	1019.2605	510.1339	1002.2300	501.6187	1001.2452	501.1263	R	303.3807	152.1940	286.3502	143.6788			2
10							K	147.1950	74.1012	130.1645	65.5859			1

Average mass of neutral peptide Mr(calc): 1164.4406 **Fixed modifications:** Carbamidomethyl (C) (apply to specified residues or termini only) **Ions Score:** 14 **Expect:** 2.5e+002 **Matches :** 4/88 fragment ions using 7 most intense peaks

Peptide View

MS/MS Fragmentation of **EITALAPSTMK**

Found in **gi|28252** in **NCBInr_human**, unnamed protein product [Homo sapiens]

Match to Query 1158: 1177.994618 from(590.004700,2+)

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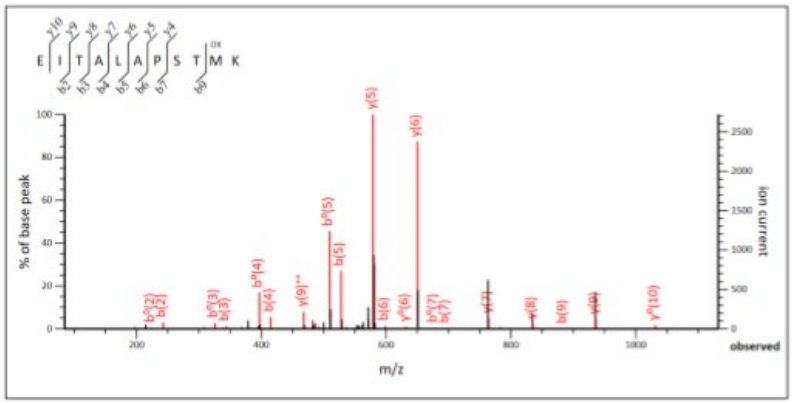


#	b	b^{++}	b^0	b^{0++}	Seq.	y	y^{++}	y^*	y^{*++}	y^0	y^{0++}	#
1	130.1214	65.5644	112.1061	56.5568	E							11
2	***243.2790***	122.1432	225.2637	113.1356	I	1049.2618	525.1346	1032.2313	516.6193	1031.2465	516.1269	10
3	***344.3829***	172.6951	326.3676	163.6875	T	**936.1042**	468.5558	919.0737	460.0405	918.0889	459.5481	9
4	***415.4608***	208.2341	397.4455	199.2265	A	**835.0003**	418.0038	817.9698	409.4886	816.9850	408.9962	8
5	***528.6184***	264.8129	510.6031	255.8053	L	**763.9224**	382.4649	746.8919	373.9496	745.9071	373.4572	7
6	***599.6963***	300.3518	581.6810	291.3442	A	**650.7648**	325.8861	633.7343	317.3708	632.7495	316.8784	6
7	***696.8115***	348.9094	678.7962	339.9018	P	**579.6869**	290.3471	562.6564	281.8319	561.6716	281.3395	5
8	783.8888	392.4481	765.8735	383.4405	S	**482.5717**	241.7895	465.5412	233.2743	464.5564	232.7819	4
9	***884.9927***	443.0000	866.9774	433.9924	T	395.4944	198.2509	378.4639	189.7356	377.4791	189.2432	3
10	***1032.1882***	516.5978	1014.1729	507.5902	M	294.3905	147.6989	277.3600	139.1837			2
11					K	147.1950	74.1012	130.1645	65.5859			1

Average mass of neutral peptide Mr(calc): 1177.3683 **Fixed modifications:** Carbamidomethyl (C) (apply to specified residues or termini only) **Variable modifications: M10 :** Oxidation (M), with neutral losses 0.0000(shown in table), 64.1069 **Ions Score:** 53 **Expect:** 0.026 **Matches :** 26/152 fragment ions using 45 most intense peaks

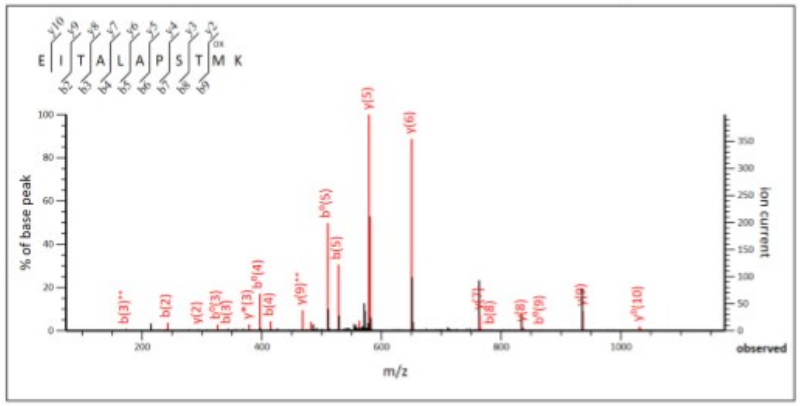
Peptide View

MS/MS Fragmentation of **EITALAPSTMK**

Found in **gi|28252** in **NCBInr_human**, unnamed protein product [Homo sapiens]

Match to Query 1161: 1178.397084 from(590.205933,2+)

Title: spectrumId=1483 Filter=ITMS + c NSI d Full ms2 590.21@cid35.00 [150.00-1195.00] PeakProcessing=continuous Polarity=positive ScanMode=MassScan TimeInMinutes=10.255660 acqNumber=1483



#	b	b^{++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y*	y*$^{++}$	y^{0}	y^{0++}	#
1	130.1214	65.5644	112.1061	56.5568	E							11
2	243.2790	122.1432	225.2637	113.1356	I	1049.2618	525.1346	1032.2313	516.6193	1031.2465	516.1269	10
3	344.3829	172.6951	326.3676	163.6875	T	*936.1042*	468.5558	919.0737	460.0405	918.0889	459.5481	9
4	415.4608	208.2341	397.4455	199.2265	A	*835.0003*	418.0038	817.9698	409.4886	816.9850	408.9962	8
5	528.6184	264.8129	510.6031	255.8053	L	*763.9224*	382.4649	746.8919	373.9496	745.9071	373.4572	7
6	599.6963	300.3518	581.6810	291.3442	A	*650.7648*	325.8861	633.7343	317.3708	632.7495	316.8784	6
7	696.8115	348.9094	678.7962	339.9018	P	*579.6869*	290.3471	562.6564	281.8319	561.6716	281.3395	5
8	783.8888	392.4481	765.8735	383.4405	S	*482.5717*	241.7895	465.5412	233.2743	464.5564	232.7819	4
9	884.9927	443.0000	866.9774	433.9924	T	*395.4944*	198.2509	378.4639	189.7356	377.4791	189.2432	3
10	1032.1882	516.5978	1014.1729	507.5902	M	*294.3905*	147.6989	277.3600	139.1837			2
11					K	147.1950	74.1012	130.1645	65.5859			1

Average mass of neutral peptide Mr(calc): 1177.3683 **Fixed modifications:** Carbamidomethyl (C) (apply to specified residues or termini only) **Variable modifications: M10 :** Oxidation (M), with neutral losses 0.0000(shown in table), 64.1069 **Ions Score:** 40 **Expect:** 0.5 **Matches :** 29/152 fragment ions using 69 most intense peaks

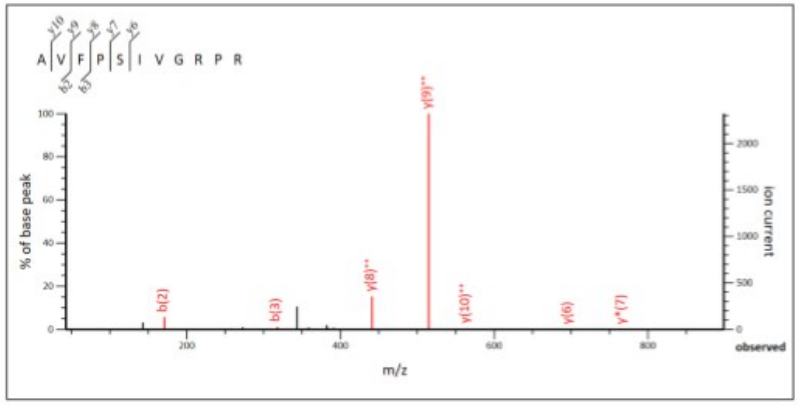
Peptide View

MS/MS Fragmentation of **AVFPSIVGRPR**

Found in **gi|28252** in **NCBInr_human**, unnamed protein product [Homo sapiens]

Match to Query 303: 1197.653121 from(400.225098,3+)

Title: spectrumId=1651 Filter=ITMS + c NSI d Full ms2 400.23@cid35.00 [100.00-815.00] PeakProcessing=continuous Polarity=positive ScanMode=MassScan TimeInMinutes=12.346508 acqNumber=1651



#	b	b^{++}	b*	b*$^{++}$	b^{0}	b^{0++}	Seq.	y	y^{++}	y*	y*$^{++}$	y^{0}	y^{0++}	#
1	72.0853	36.5463					A							11
2	171.2164	86.1119					V	1128.3468	*564.6771*	1111.3163	556.1618	1110.3315	555.6694	10
3	318.3903	159.6988					F	1029.2157	*515.1115*	1012.1852	506.5963	1011.2004	506.1039	9
4	415.5055	208.2564					P	882.0418	*441.5246*	865.0113	433.0093	864.0265	432.5169	8
5	502.5828	251.7951			484.5675	242.7875	S	784.9266	392.9670	767.8961	384.4517	766.9113	383.9593	7
6	615.7404	308.3739			597.7251	299.3663	I	697.8493	349.4283	680.8188	340.9131			6
7	714.8715	357.9394			696.8562	348.9318	V	584.6917	292.8495	567.6612	284.3343			5
8	771.9228	386.4651			753.9075	377.4575	G	485.5606	243.2840	468.5301	234.7687			4
9	928.1085	464.5579	911.0780	456.0427	910.0932	455.5503	R	428.5093	214.7583	411.4788	206.2431			3
10	1025.2237	513.1155	1008.1932	504.6003	1007.2084	504.1079	P	272.3236	136.6655	255.2931	128.1502			2
11							R	175.2084	88.1079	158.1779	79.5926			1

Average mass of neutral peptide Mr(calc): 1198.4173 **Fixed modifications:** Carbamidomethyl (C) (apply to specified residues or termini only) **Ions Score:** 21 **Expect:** 28 **Matches :** 8/84 fragment ions using 7 most intense peaks

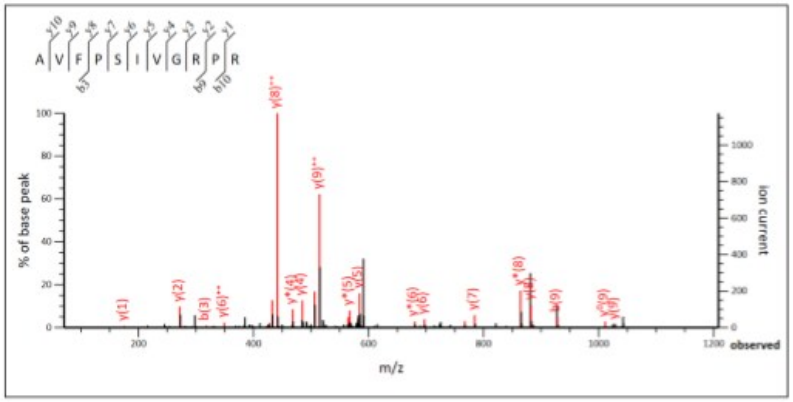
Peptide View

MS/MS Fragmentation of **AVFPSIVGRPR**

Found in **gi|28252** in **NCBInr_human**, unnamed protein product [Homo sapiens]

Match to Query 1188: 1198.806384 from(600.410583,2+)

Title: spectrumId=1642 Filter=ITMS + c NSI d Full ms2 600.41@cid35.00 [155.00-1215.00] PeakProcessing=continuous Polarity=positive ScanMode=MassScan TimeInMinutes=12.231093 acqNumber=1642



#	b	b^{++}	b*	b*$^{++}$	b^{0}	b^{0++}	Seq.	y	y^{++}	y*	y*$^{++}$	y^{0}	y^{0++}	#
1	72.0853	36.5463					A							11
2	171.2164	86.1119					V	1128.3468	564.6771	1111.3163	556.1618	1110.3315	555.6694	10
3	318.3903	159.6988					F	1029.2157	515.1115	1012.1852	506.5963	1011.2004	506.1039	9
4	415.5055	208.2564					P	882.0418	441.5246	865.0113	433.0093	864.0265	432.5169	8
5	502.5828	251.7951			484.5675	242.7875	S	784.9266	392.9670	767.8961	384.4517	766.9113	383.9593	7
6	615.7404	308.3739			597.7251	299.3663	I	697.8493	349.4283	680.8188	340.9131			6
7	714.8715	357.9394			696.8562	348.9318	V	584.6917	292.8495	567.6612	284.3343			5
8	771.9228	386.4651			753.9075	377.4575	G	485.5606	243.2840	468.5301	234.7687			4
9	928.1085	464.5579	911.0780	456.0427	910.0932	455.5503	R	428.5093	214.7583	411.4788	206.2431			3
10	1025.2237	513.1155	1008.1932	504.6003	1007.2084	504.1079	P	272.3236	136.6655	255.2931	128.1502			2
11							R	175.2084	88.1079	158.1779	79.5926			1

Average mass of neutral peptide Mr(calc): 1198.4173 **Fixed modifications:** Carbamidomethyl (C) (apply to specified residues or termini only) **Ions Score:** 52 **Expect:** 0.026 **Matches :** 30/84 fragment ions using 73 most intense peaks

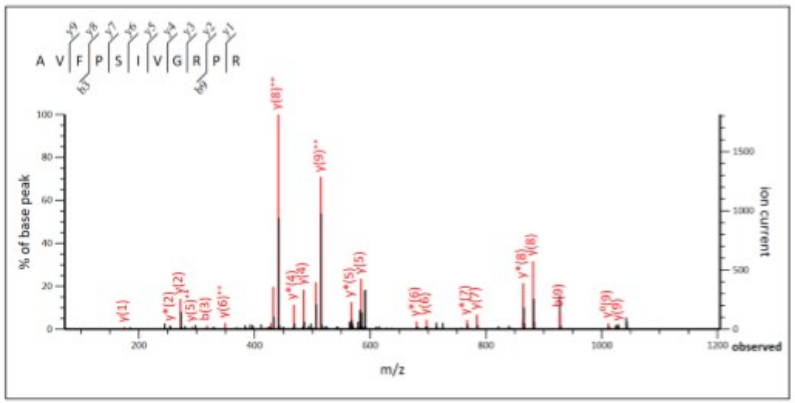
Peptide View

MS/MS Fragmentation of **AVFPSIVGRPR**

Found in **gi|28252** in **NCBInr_human**, unnamed protein product [Homo sapiens]

Match to Query 1189: 1199.478382 from(600.746582,2+)

Title: spectrumId=1661 Filter=ITMS + c NSI d Full ms2 600.75@cid35.00 [155.00-1215.00] PeakProcessing=continuous Polarity=positive ScanMode=MassScan TimeInMinutes=12.472018 acqNumber=1661



#	b	b^{++}	b*	b*$^{++}$	b^{0}	b^{0++}	Seq.	y	y^{++}	y*	y*$^{++}$	y^{0}	y^{0++}	#
1	72.0853	36.5463					A							11
2	171.2164	86.1119					V	1128.3468	564.6771	1111.3163	556.1618	1110.3315	555.6694	10
3	318.3903	159.6988					F	1029.2157	515.1115	1012.1852	506.5963	1011.2004	506.1039	9
4	415.5055	208.2564					P	882.0418	441.5246	865.0113	433.0093	864.0265	432.5169	8
5	502.5828	251.7951			484.5675	242.7875	S	784.9266	392.9670	767.8961	384.4517	766.9113	383.9593	7
6	615.7404	308.3739			597.7251	299.3663	I	697.8493	349.4283	680.8188	340.9131			6
7	714.8715	357.9394			696.8562	348.9318	V	584.6917	292.8495	567.6612	284.3343			5
8	771.9228	386.4651			753.9075	377.4575	G	485.5606	243.2840	468.5301	234.7687			4
9	928.1085	464.5579	911.0780	456.0427	910.0932	455.5503	R	428.5093	214.7583	411.4788	206.2431			3
10	1025.2237	513.1155	1008.1932	504.6003	1007.2084	504.1079	P	272.3236	136.6655	255.2931	128.1502			2
11							R	175.2084	88.1079	158.1779	79.5926			1

Average mass of neutral peptide Mr(calc): 1198.4173 **Fixed modifications:** Carbamidomethyl (C) (apply to specified residues or termini only) **Ions Score:** 61 **Expect:** 0.0047 **Matches :** 29/84 fragment ions using 56 most intense peaks

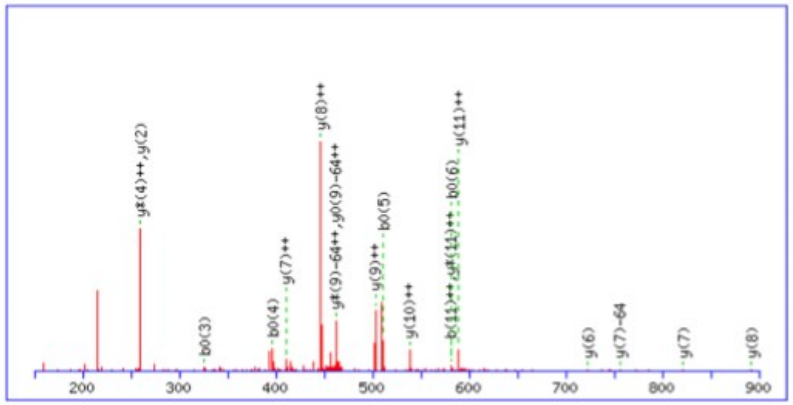
Peptide View

MS/MS Fragmentation of **EITALAPSTMKIK**

Found in **gi|28252** in **NCBInr_human**, unnamed protein product [Homo sapiens]

Match to Query 834: 1419.749526 from(474.257233,3+)

Title: spectrumId=1490 Filter=ITMS + c NSI d Full ms2 474.26@cid35.00 [120.00-960.00] PeakProcessing=continuous Polarity=positive ScanMode=MassScan TimeInMinutes=10.338302 acqNumber=1490



#	b	b^{++}	b^*	b^{*++}	b^0	b^{0++}	Seq.	y	y^{++}	y^*	y^{*++}	y^0	y^{0++}	#
1	130.1214	65.5644			112.1061	56.5568	E							13
2	243.2790	122.1432			225.2637	113.1356	I	1290.5917	645.7995	1273.5612	637.2843	1272.5764	636.7919	12
3	344.3829	172.6951			326.3676	163.6875	T	1177.4341	***589.2207***	1160.4036	580.7055	1159.4188	580.2131	11
4	415.4608	208.2341			397.4455	199.2265	A	1076.3302	***538.6688***	1059.2997	530.1535	1058.3149	529.6611	10
5	528.6184	264.8129			510.6031	255.8053	L	1005.2523	***503.1298***	988.2218	494.6146	987.2370	494.1222	9
6	599.6963	300.3518			581.6810	291.3442	A	***892.0947***	***446.5510***	875.0642	438.0358	874.0794	437.5434	8
7	696.8115	348.9094			678.7962	339.9018	P	***821.0168***	***411.0121***	803.9863	402.4968	803.0015	402.0044	7
8	783.8888	392.4481												

Average mass of neutral peptide Mr(calc): 1418.6982 **Fixed modifications:** Carbamidomethyl (C) (apply to specified residues or termini only) **Variable modifications: M10 :** Oxidation (M), with neutral losses 0.0000(shown in table), 64.1069 **Ions Score:** 17 **Expect:** 96 **Matches :** 19/184 fragment ions using 40 most intense peaks

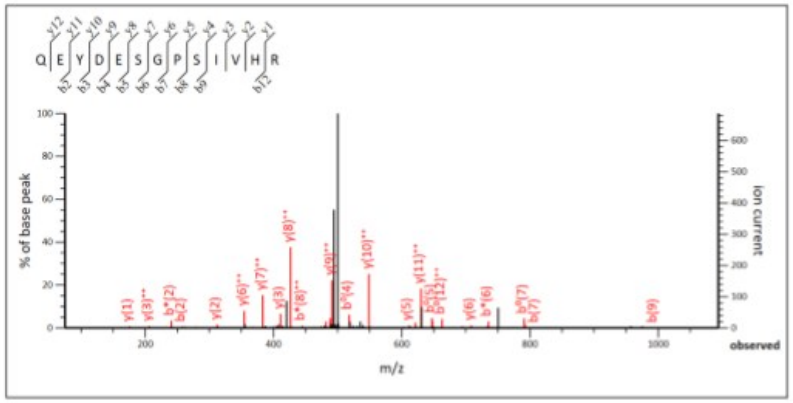
Peptide View

MS/MS Fragmentation of **QEYDESGPSIVHR**

Found in **gi|28252** in **NCBInr_human**, unnamed protein product [Homo sapiens]

Match to Query 898: 1517.233962 from(506.752045,3+)

Title: spectrumId=1425 Filter=ITMS + c NSI d Full ms2 506.75@cid35.00 [125.00-1025.00] PeakProcessing=continuous Polarity=positive ScanMode=MassScan TimeInMinutes=9.510245 acqNumber=1425



#	b	b^{++}	b^*	b^{*++}	b^0	b^{0++}	Seq.	y	y^{++}	y^*	y^{*++}	y^0	y^{0++}	#
1	129.1366	65.0720	112.1061	56.5567			Q							13
2	**258.2506**	129.6290	241.2201	121.1137	240.2353	120.6214	E	1389.4462	***695.2268***	1372.4157	686.7115	1371.4309	686.2191	12
3	421.4239	211.2156	404.3934	202.7004	403.4086	202.2080	Y	1260.3322	***630.6698***	1243.3017	622.1545	1242.3169	621.6621	11
4	536.5113	268.7593	519.4808	260.2441	518.4960	259.7517	D	1097.1589	***549.0831***	1080.1284	540.5679	1079.1436	540.0755	10
5	665.6253	333.3163	648.5948	324.8011	647.6100	324.3087	E	982.0715	***491.5394***	965.0410	483.0242	964.0562	482.5318	9
6	752.7026	376.8550	735.6721	368.3397	734.6873	367.8474	S	852.9575	***426.9824***	835.9270	418.4672	834.9422	417.9748	8
7	**809.7539**	405.3806	792.7234	396.8654	791.7386	396.3730	G	765.8802	***383.4438***	748.8497	374.9285	747.8649	374.4361	7
8	906.8691	453.9382	889.8386	445.4230	888.8538	444.9306	P	***708.8289***	***354.9181***	691.7984	346.4029	690.8136	345.9105	6
9	**993.9464**	497.4769	976.9159	488.9616	975.9311	488.4693	S	***611.7137***	306.3605	594.6832	297.8453	593.6984	297.3529	5
10	1107.1040	554.0557	1090.0735	545.5404	1089.0887	545.0481	I	524.6364	***262.8219***	507.6059	254.3066			4
11	1206.2351	603.6212	1189.2046	595.1060	1188.2198	594.6136	V	***411.4788***	***206.2431***	394.4483	197.7278			3
12	1343.3744	672.1909	1326.3439	663.6756	1325.3591	663.1833	H	***312.3477***	156.6775	295.3172	148.1623			2
13							R	***175.2084***	88.1079	158.1779	79.5926			1

Average mass of neutral peptide Mr(calc): 1516.5679 **Fixed modifications:** Carbamidomethyl (C) (apply to specified residues or termini only) **Ions Score:** 64 **Expect:** 0.0015 **Matches :** 37/134 fragment ions using 54 most intense peaks

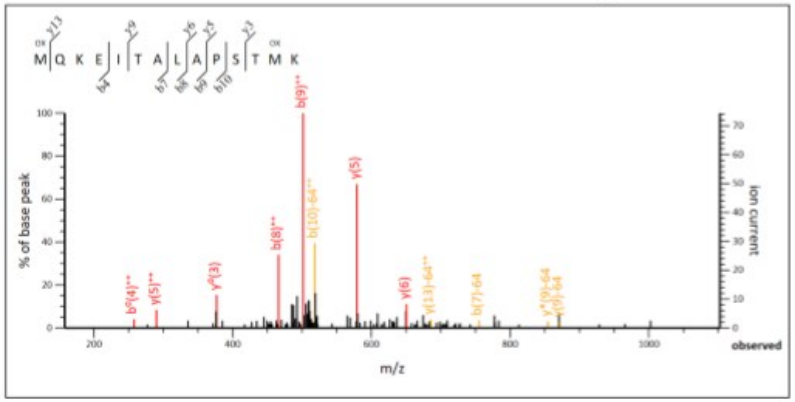
Peptide View

MS/MS Fragmentation of **MQKEITALAPSTMK**

Found in **gi|28252** in **NCBInr_human**, unnamed protein product [Homo sapiens]

Match to Query 965: 1581.262740 from(528.094971,3+)

Title: spectrumId=1457 Filter=ITMS + c NSI d Full ms2 528.09@cid35.00 [135.00-1070.00] PeakProcessing=continuous Polarity=positive ScanMode=MassScan TimeInMinutes=9.924432 acqNumber=1457



#	b	b**	b*	b***	b°	b°**	Seq.	y	y**	y*	y***	y°	y°**	#
1	148.2029	74.6051					M							14
2	276.3321	138.6697	259.3016	130.1545			Q	1434.6773	717.8423	1417.6468	709.3271	1416.6620	708.8347	13
3	404.5044	202.7559	387.4739	194.2406			K	1306.5481	653.7777	1289.5176	645.2625	1288.5328	644.7701	12
4	533.6184	267.3129	516.5879	258.7976	515.6031	258.3053	E	1178.3758	589.6916	1161.3453	581.1763	1160.3605	580.6839	11
5	646.7760	323.8917	629.7455	315.3764	628.7607	314.8841	I	1049.2618	525.1346	1032.2313	516.6193	1031.2465	516.1269	10
6	747.8799	374.4436	730.8494	365.9284	729.8646	365.4360	T	936.1042	468.5558	919.0737	460.0405	918.0889	459.5481	9
7	818.9578	409.9826	801.9273	401.4673	800.9425	400.9750	A	835.0003	418.0038	817.9698	409.4886	816.9850	408.9962	8
8	932.1154	*466.5614*	915.0849	458.0461	914.1001	457.5538	L	763.9224	382.4649	746.8919	373.9496	745.9071	373.4572	7
9	1003.1933	*502.1003*	986.1628	493.5851	985.1780	493.0927	A	*650.7648*	325.8861	633.7343	317.3708	632.7495	316.8784	6
10	1100.3085	550.6579	1083.2780	542.1427	1082.2932	541.6503	P	*579.6869*	290.3471	562.6564	281.8319	561.6716	281.3395	5
11	1187.3858	594.1966	1170.3553	585.6813	1169.3705	585.1890	S	482.5717	241.7895	465.5412	233.2743	464.5564	232.7819	4
12	1288.4897	644.7485	1271.4592	636.2333	1270.4744	635.7409	T	395.4944	198.2509	378.4639	189.7356	377.4791	189.2432	3
13	1435.6852	718.3463	1418.6547	709.8310	1417.6699	709.3387	M	294.3905	147.6989	277.3600	139.1837			2
14							K	147.1950	74.1012	130.1645	65.5859			1

Average mass of neutral peptide Mr(calc): 1580.8654 **Fixed modifications:** Carbamidomethyl (C) (apply to specified residues or termini only) **Variable modifications:** **M1 :** Oxidation (M), with neutral losses 0.0000(shown in table), 64.1069 **M13 :** Oxidation (M), with neutral losses 0.0000(shown in table), 64.1069 **Ions Score:** 2 **Expect:** 2.7e+003 **Matches :** 15/284 fragment ions using 23 most intense peaks

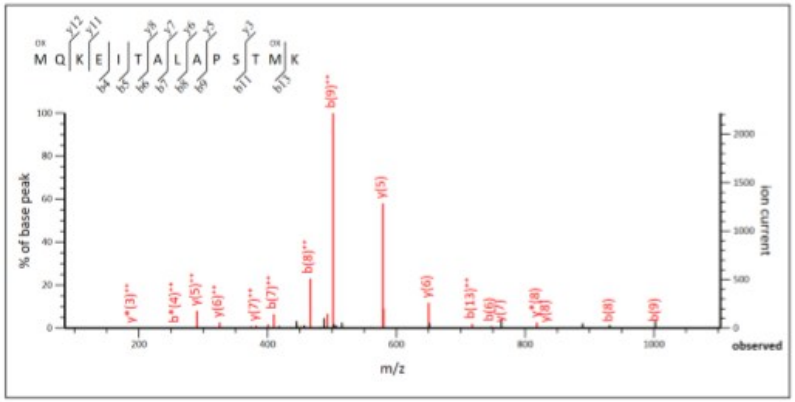
Peptide View

MS/MS Fragmentation of **MQKEITALAPSTMK**

Found in **gi|28252** in **NCBInr_human**, unnamed protein product [Homo sapiens]

Match to Query 966: 1581.494184 from(528.172119,3+)

Title: spectrumId=1393 Filter=ITMS + c NSI d Full ms2 528.17@cid35.00 [135.00-1070.00] PeakProcessing=continuous Polarity=positive ScanMode=MassScan TimeInMinutes=9.098173 acqNumber=1393



#	b	b**	b*	b***	b°	b°**	Seq.	y	y**	y*	y***	y°	y°**	#
1	148.2029	74.6051					M							14
2	276.3321	138.6697	259.3016	130.1545			Q	1434.6773	*717.8423*	1417.6468	709.3271	1416.6620	708.8347	13
3	404.5044	202.7559	387.4739	194.2406			K	1306.5481	653.7777	1289.5176	645.2625	1288.5328	644.7701	12
4	533.6184	267.3129	516.5879	258.7976	515.6031	258.3053	E	1178.3758	589.6916	1161.3453	581.1763	1160.3605	580.6839	11
5	646.7760	323.8917	629.7455	315.3764	628.7607	314.8841	I	1049.2618	525.1346	1032.2313	516.6193	1031.2465	516.1269	10
6	*747.8799*	*374.4436*	730.8494	365.9284	729.8646	365.4360	T	936.1042	468.5558	919.0737	460.0405	918.0889	459.5481	9
7	*818.9578*	*409.9826*	801.9273	401.4673	800.9425	400.9750	A	*835.0003*	418.0038	817.9698	409.4886	816.9850	408.9962	8
8	*932.1154*	*466.5614*	915.0849	458.0461	914.1001	457.5538	L	*763.9224*	*382.4649*	746.8919	373.9496	745.9071	373.4572	7
9	*1003.1933*	*502.1003*	986.1628	493.5851	985.1780	493.0927	A	*650.7648*	*325.8861*	633.7343	317.3708	632.7495	316.8784	6
10	1100.3085	550.6579	1083.2780	542.1427	1082.2932	541.6503	P	*579.6869*	*290.3471*	562.6564	281.8319	561.6716	281.3395	5
11	1187.3858	*594.1966*	1170.3553	585.6813	1169.3705	585.1890	S	482.5717	241.7895	465.5412	233.2743	464.5564	232.7819	4
12	1288.4897	*644.7485*	1271.4592	636.2333	1270.4744	635.7409	T	395.4944	198.2509	378.4639	189.7356	377.4791	189.2432	3
13	1435.6852	*718.3463*	1418.6547	709.8310	1417.6699	709.3387	M	294.3905	147.6989	277.3600	139.1837			2
14							K	147.1950	74.1012	130.1645	65.5859			1

Average mass of neutral peptide Mr(calc): 1580.8654 **Fixed modifications:** Carbamidomethyl (C) (apply to specified residues or termini only) **Variable modifications:** **M1 :** Oxidation (M), with neutral losses 0.0000(shown in table), 64.1069 **M13 :** Oxidation (M), with neutral losses 0.0000(shown in table), 64.1069 **Ions Score:** 45 **Expect:** 0.15 **Matches :** 39/284 fragment ions using 40 most intense peaks

Peptide View

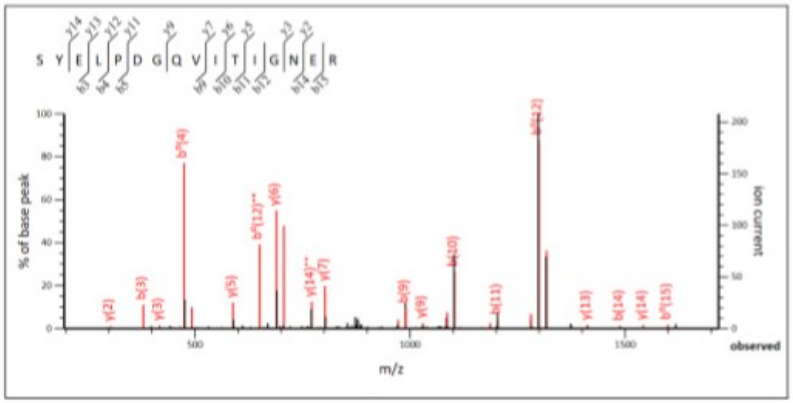
MS/MS Fragmentation of **SYELPDGQVITIGNER**

Found in **gi|28252** in **NCBInr_human**, unnamed protein product [Homo sapiens]

Match to Query 1724: 1790.412708 from(896.213745,2+)

Title: spectrumId=1938 Filter=ITMS + c NSI d Full ms2 896.21@cid35.00 [235.00-1805.00] PeakProcessing=continuous Polarity=positive

ScanMode=MassScan TimeInMinutes=16.012137 acqNumber=1938



#	b	b**	b*	b***	b^0	b^{0**}	Seq.	y	y**	y*	y***	y^0	y^{0**}	#
1	88.0847	44.5460			70.0694	35.5384	S							16
2	251.2580	126.1327			233.2427	117.1251	V	1704.8545	852.9309	1687.8240	844.4157	1686.8392	843.9233	15
3	**380.3720**	190.6897			362.3567	181.6821	E	***1541.6812***	**771.3443**	1524.6507	762.8290	1523.6659	762.3366	14
4	**493.5296**	247.2685			475.5143	238.2609	L	***1412.5672***	**706.7873**	1395.5367	698.2720	1394.5519	697.7796	13
5	590.6448	295.8261			572.6295	286.8185	P	***1299.4096***	**650.2085**	1282.3791	641.6932	1281.3943	641.2008	12
6	705.7322	353.3698			687.7169	344.3622	D	1202.2944	601.6509	1185.2639	593.1356	1184.2791	592.6432	11
7	762.7835	381.8954			744.7682	372.8878	G	1087.2070	544.1072	1070.1765	535.5919	1069.1917	535.0995	10
8	890.9127	445.9600	873.8822	437.4448	872.8974	436.9524	Q	***1030.1557***	515.5815	1013.1252	507.0663	1012.1404	506.5739	9
9	**990.0438**	495.5256	973.0133	487.0103	972.0285	486.5180	V	902.0265	451.5169	884.9960	443.0017	884.0112	442.5093	8
10	**1103.2014**	552.1044	1086.1709	543.5891	1085.1861	543.0968	I	***802.8954***	401.9514	785.8649	393.4361	784.8801	392.9437	7
11	**1204.3053**	602.6563	1187.2748	594.1411	1186.2900	593.6487	T	***689.7378***	345.3726	672.7073	336.8573	671.7225	336.3649	6
12	**1317.4629**	659.2351	1300.4324	650.7199	1299.4476	650.2275	I	***588.6339***	294.8206	571.6034	286.3054	570.6186	285.8130	5
13	1374.5142	687.7608	1357.4837	679.2455	1356.4989	678.7532	G	***475.4763***	238.2418	458.4458	229.7266	457.4610	229.2342	4
14	**1488.6168**	744.8121	1471.5863	736.2968	1470.6015	735.8045	N	***418.4250***	209.7162	401.3945	201.2009	400.4097	200.7085	3
15	1617.7308	809.3691	1600.7003	800.8538	1599.7155	800.3615	E	***304.3224***	152.6649	287.2919	144.1496	286.3071	143.6572	2
16							R	175.2084	88.1079	158.1779	79.5926			1

Average mass of neutral peptide Mr(calc): 1790.9243 **Fixed modifications:** Carbamidomethyl (C) (apply to specified residues or termini only) **Ions Score:** 58 **Expect:** 0.0048 **Matches :** 31/164 fragment ions using 50 most intense peaks

Peptide View

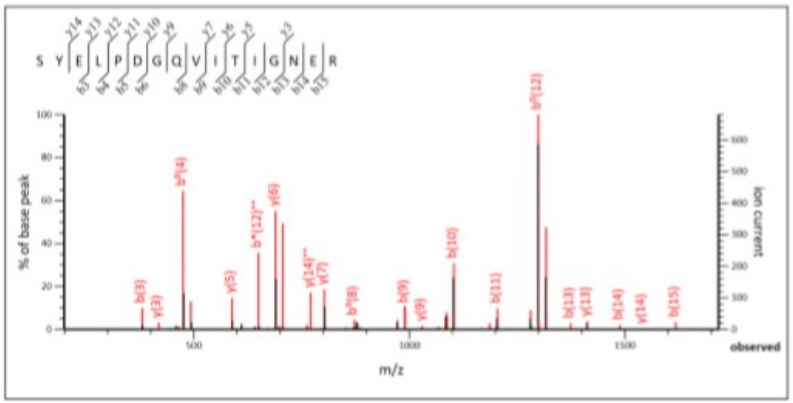
MS/MS Fragmentation of **SYELPDGQVITIGNER**

Found in **gi|28252** in **NCBInr_human**, unnamed protein product [Homo sapiens]

Match to Query 1725: 1790.426624 from(896.220703,2+)

Title: spectrumId=1915 Filter=ITMS + c NSI d Full ms2 896.22@cid35.00 [235.00-1805.00] PeakProcessing=continuous Polarity=positive

ScanMode=MassScan TimeInMinutes=15.703047 acqNumber=1915



#	b	b**	b*	b***	b^0	b^{0**}	Seq.	y	y**	y*	y***	y^0	y^{0**}	#
1	88.0847	44.5460			70.0694	35.5384	S							16
2	251.2580	126.1327			233.2427	117.1251	V	1704.8545	852.9309	1687.8240	844.4157	1686.8392	843.9233	15
3	***380.3720***	190.6897			362.3567	181.6821	E	**1541.6812**	**771.3443**	1524.6507	762.8290	1523.6659	762.3366	14
4	***493.5296***	247.2685			475.5143	238.2609	L	**1412.5672**	**706.7873**	1395.5367	698.2720	1394.5519	697.7796	13
5	***590.6448***	295.8261			572.6295	286.8185	P	**1299.4096**	**650.2085**	1282.3791	641.6932	1281.3943	641.2008	12
6	***705.7322***	353.3698			687.7169	344.3622	D	1202.2944	601.6509	1185.2639	593.1356	1184.2791	592.6432	11
7	***762.7835***	381.8954			744.7682	372.8878	G	**1087.2070**	544.1072	1070.1765	535.5919	1069.1917	535.0995	10
8	890.9127	445.9600	873.8822	437.4448	872.8974	436.9524	Q	**1030.1557**	515.5815	1013.1252	507.0663	1012.1404	506.5739	9
9	***990.0438***	495.5256	973.0133	487.0103	972.0285	486.5180	V	902.0265	451.5169	884.9960	443.0017	884.0112	442.5093	8
10	***1103.2014***	552.1044	1086.1709	543.5891	1085.1861	543.0968	I	**802.8954**	401.9514	785.8649	393.4361	784.8801	392.9437	7
11	***1204.3053***	602.6563	1187.2748	594.1411	1186.2900	593.6487	T	**689.7378**	345.3726	672.7073	336.8573	671.7225	336.3649	6
12	***1317.4629***	659.2351	1300.4324	650.7199	1299.4476	650.2275	I	**588.6339**	294.8206	571.6034	286.3054	570.6186	285.8130	5
13	***1374.5142***	687.7608	1357.4837	679.2455	1356.4989	678.7532	G	**475.4763**	238.2418	458.4458	229.7266	457.4610	229.2342	4
14	***1488.6168***	744.8121	1471.5863	736.2968	1470.6015	735.8045	N	**418.4250**	209.7162	401.3945	201.2009	400.4097	200.7085	3
15	***1617.7308***	809.3691	1600.7003	800.8538	1599.7155	800.3615	E	304.3224	152.6649	287.2919	144.1496	286.3071	143.6572	2
16							R	175.2084	88.1079	158.1779	79.5926			1

Average mass of neutral peptide Mr(calc): 1790.9243 **Fixed modifications:** Carbamidomethyl (C) (apply to specified residues or termini only) **Ions Score:** 84 **Expect:** 1.1e-005 **Matches :** 42/164 fragment ions using 62 most intense peaks

Peptide View

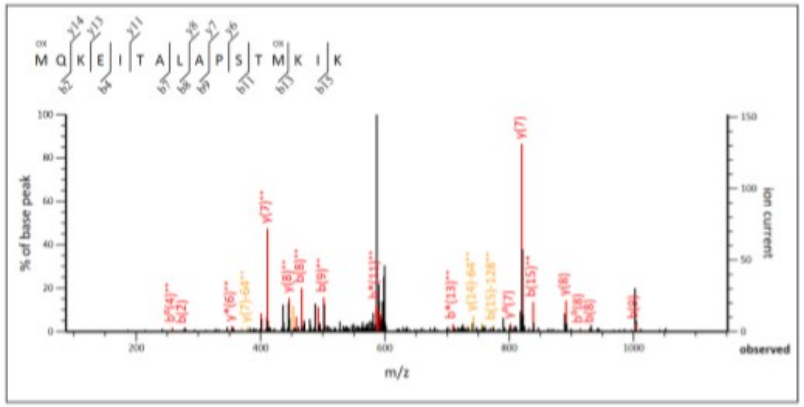
MS/MS Fragmentation of **MQKEITALAPSTMKIK**

Found in **gi|28252** in **NCBInr_human**, unnamed protein product [Homo sapiens]

Match to Query 1212: 1822.094769 from(608.372314,3+)

Title: spectrumId=1488 Filter=ITMS + c NSI d Full ms2 608.37@cid35.00 [155.00-1230.00] PeakProcessing=continuous Polarity=positive

ScanMode=MassScan TimeInMinutes=10.319560 acqNumber=1488



#	b	b++	b*	b*++	b°	b°++	Seq.	y	y++	y*	y*++	y°	y°++	#
1	148.2029	74.6051					M							16
2	276.3321	138.6697	259.3016	130.1545			Q	1676.0072	838.5073	1658.9767	829.9920	1657.9919	829.4996	15
3	404.5044	202.7559	387.4739	194.2406			K	1547.8780	774.4427	1530.8475	765.9274	1529.8627	765.4350	14
4	533.6184	267.3129	516.5879	258.7976	515.6031	258.3053	E	1419.7057	710.3565	1402.6752	701.8413	1401.6904	701.3489	13
5	646.7760	323.8917	629.7455	315.3764	628.7607	314.8841	I	1290.5917	645.7995	1273.5612	637.2843	1272.5764	636.7919	12
6	747.8799	374.4436	730.8494	365.9284	729.8646	365.4360	T	1177.4341	589.2207	1160.4036	580.7055	1159.4188	580.2131	11
7	818.9578	409.9826	801.9273	401.4673	800.9425	400.9750	A	1076.3302	538.6688	1059.2997	530.1535	1058.3149	529.6611	10
8	932.1154	466.5614	915.0849	458.0461	914.1001	457.5538	L	1005.2523	503.1298	988.2218	494.6146	987.2370	494.1222	9
9	1003.1933	502.1003	986.1628	493.5851	985.1780	493.0927	A	892.0947	446.5510	875.0642	438.0358	874.0794	437.5434	8
10	1100.3085	550.6579	1083.2780	542.1427	1082.2932	541.6503	P	821.0168	411.0121	803.9863	402.4968	803.0015	402.0044	7
11	1187.3858	594.1966	1170.3553	585.6813	1169.3705	585.1890	S	723.9016	362.4545	706.8711	353.9392	705.8863	353.4468	6
12	1288.4897	644.7485	1271.4592	636.2333	1270.4744	635.7409	T	636.8243	318.9158	619.7938	310.4006	618.8090	309.9082	5
13	1435.6852	718.3463	1418.6547	709.8310	1417.6699	709.3387	M	535.7204	268.3639	518.6899	259.8486			4
14	1563.8575	782.4324	1546.8270	773.9172	1545.8422	773.4248	K	388.5249	194.7661	371.4944	186.2509			3
15	1677.0151	839.0112	1659.9846	830.4960	1658.9998	830.0036	I	260.3526	130.6800	243.3221	122.1647			2
16							K	147.1950	74.1012	130.1645	65.5859			1

Average mass of neutral peptide Mr(calc): 1822.1953 **Fixed modifications:** Carbamidomethyl (C) (apply to specified residues or termini only) **Variable modifications: M1 :** Oxidation (M), with neutral losses 0.0000(shown in table), 64.1069 **M13 :** Oxidation (M), with neutral losses 0.0000(shown in table), 64.1069 **Ions Score:** 15 **Expect:** 1.4e+002 **Matches :** 41/316 fragment ions using 76 most intense peaks

Peptide View

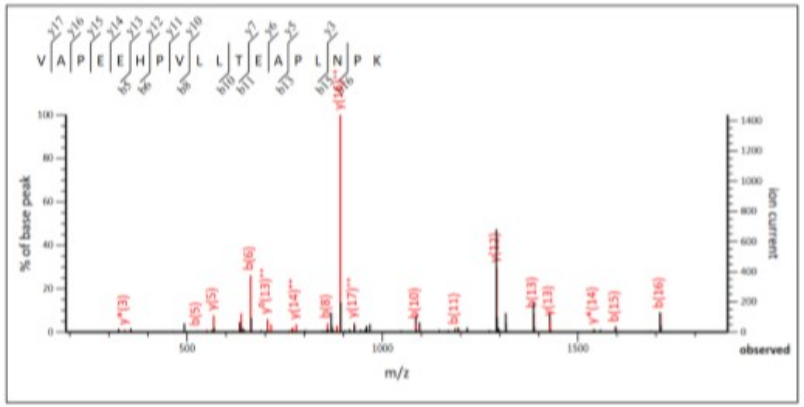
MS/MS Fragmentation of **VAPEEHPVLLTEAPLNPK**

Found in **gi|28252** in **NCBInr_human**, unnamed protein product [Homo sapiens]

Match to Query 1759: 1953.677844 from(977.846313,2+)

Title: spectrumId=1692 Filter=ITMS + c NSI d Full ms2 977.85@cid35.00 [255.00-1970.00] PeakProcessing=continuous Polarity=positive

ScanMode=MassScan TimeInMinutes=12.864683 acqNumber=1692



#	b	b++	b*	b*++	b°	b°++	Seq.	y	y++	y*	y*++	y°	y°++	#
1	100.1385	50.5729					V							18
2	171.2164	86.1119					A	1856.1033	928.5553	1839.0728	920.0401	1838.0880	919.5477	17
3	268.3316	134.6695					P	1785.0254	893.0164	1767.9949	884.5011	1767.0101	884.0087	16
4	397.4456	199.2265			379.4303	190.2189	E	1687.9192	844.4633	1670.8797	835.9435	1669.8949	835.4511	15
5	526.5596	263.7835			508.5443	254.7759	E	1558.7962	779.9018	1541.7657	771.3865	1540.7809	770.8941	14
6	663.6989	332.3531			645.6836	323.3455	H	1429.6822	715.3448	1412.6517	706.8295	1411.6669	706.3371	13
7	760.8141	380.9107			742.7988	371.9031	P	1292.5429	646.7751	1275.5124	638.2599	1274.5276	637.7675	12
8	859.9452	430.4763			841.9299	421.4687	V	1195.4277	598.2175	1178.3972	589.7023	1177.4124	589.2099	11
9	973.1028	487.0551			955.0875	478.0475	L	1096.2966	548.6520	1079.2661	540.1367	1078.2813	539.6443	10
10	1086.2604	543.6339			1068.2451	534.6263	L	983.1390	492.0732	966.1085	483.5579	965.1237	483.0655	9
11	1187.3641	594.1858			1169.3490	585.1782	T	869.9814	435.4944	852.9509	426.9791	851.9661	426.4867	8
12	1316.4783	658.7428			1298.4630	649.7352	E	768.8775	384.9424	751.8470	376.4272	750.8622	375.9348	7
13	1387.5562	694.2818			1369.5409	685.2742	A	639.7635	320.3854	622.7330	311.8702			6
14	1484.6714	742.8394			1466.6561	733.8318	P	568.6856	284.8465	551.6551	276.3312			5
15	1597.8290	799.4182			1579.8137	790.4106	L	471.5704	236.2889	454.5399	227.7736			4
16	1711.9316	856.4695	1694.9011	847.9542	1693.9163	847.4619	N	358.4120	179.7101	341.3823	171.1948			3
17	1809.0468	905.0271	1792.0163	896.5118	1791.0315	896.0195	P	244.3107	122.6589	227.2797	114.1435			2
18							K	147.1950	74.1012	130.1645	65.5859			1

Average mass of neutral peptide Mr(calc): 1954.2269 **Fixed modifications:** Carbamidomethyl (C) (apply to specified residues or termini only) **Ions Score:** 41 **Expect:** 0.25 **Matches :** 35/156 fragment ions using 90 most intense peaks

Peptide View

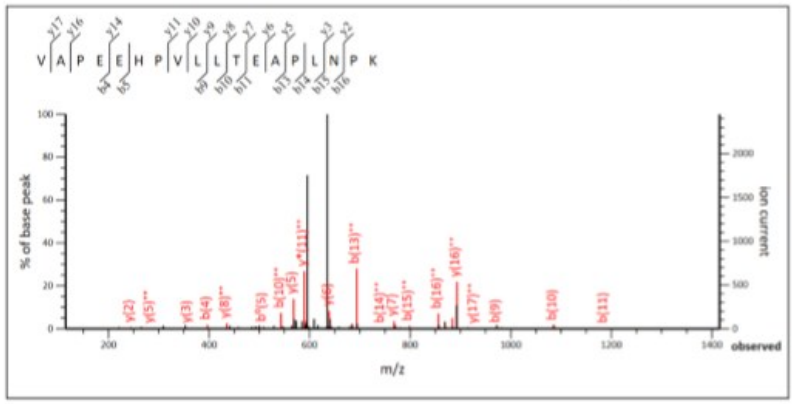
MS/MS Fragmentation of **VAPEEHPVLLTEAPLNPK**

Found in **gi|28252** in **NCBInr_human**, unnamed protein product [Homo sapiens]

Match to Query 1342: 1955.121261 from(652.714478,3+)

Title: spectrumId=1732 Filter=ITMS + c NSI d Full ms2 652.71@cid35.00 [165.00-1320.00] PeakProcessing=continuous Polarity=positive

ScanMode=MassScan TimeInMinutes=13.368062 acqNumber=1732



#	b	b**	b*	b***	b°	b°**	Seq.	y	y**	y*	y***	y°	y°**	#
1	100.1385	50.5729					V							18
2	171.2164	86.1119					A	1856.1033	**928.5553**	1839.0728	920.0401	1838.0888	919.5477	17
3	268.3316	134.6695					P	1785.0254	***893.0164***	1767.9949	884.5011	1767.0101	884.0087	16
4	**397.4456**	199.2265			379.4303	190.2189	E	1687.9102	844.4588	1670.8797	835.9435	1669.8949	835.4511	15
5	526.5596	263.7835			508.5443	254.7759	E	1558.7962	***779.9018***	1541.7657	771.3865	1540.7809	770.8941	14
6	663.6989	332.3531			645.6836	323.3455	H	1429.6822	715.3448	1412.6517	706.8295	1411.6669	706.3371	13
7	760.8141	380.9107			742.7988	371.9031	P	1292.5429	646.7751	1275.5124	638.2599	1274.5276	637.7675	12
8	859.9452	430.4763			841.9299	421.4687	V	1195.4277	598.2175	1178.3972	589.7023	1177.4124	589.2099	11
9	**973.1028**	487.0551			955.0875	478.0475	L	***1096.2966***	548.6520	1079.2661	540.1367	1078.2813	539.6443	10
10	**1086.2604**	**543.6339**			1068.2451	534.6263	L	***983.1390***	***492.0732***	966.1085	483.5579	965.1237	483.0655	9
11	**1187.3643**	**594.1858**			1169.3490	585.1782	T	***869.9814***	***435.4944***	852.9509	426.9791	851.9661	426.4867	8
12	1316.4783	658.7428			1298.4630	649.7352	E	***768.8775***	***384.9424***	751.8470	376.4272	750.8622	375.9348	7
13	1387.5562	**694.2818**			1369.5409	685.2742	A	***639.7615***	320.3854	622.7330	311.8702			6
14	1484.6714	**742.8394**			1466.6561	733.8318	P	***568.6856***	***284.8465***	551.6551	276.3312			5
15	1597.8290	**799.4182**			1579.8137	790.4106	L	471.5704	236.2889	454.5399	227.7736			4
16	1711.9316	**856.4695**	1694.9011	847.9542	1693.9163	847.4619	N	***358.4128***	179.7101	341.3823	171.1948			3
17	1809.0468	905.0271	1792.0163	896.5118	1791.0315	896.0195	P	***244.3102***	122.6588	227.2797	114.1435			2
18							K	147.1950	74.1012	130.1645	65.5859			1

Average mass of neutral peptide Mr(calc): 1954.2269 **Fixed modifications:** Carbamidomethyl (C) (apply to specified residues or termini only) **Ions Score:** 36

Expect: 1.3 **Matches :** 34/156 fragment ions using 73 most intense peaks

Peptide View

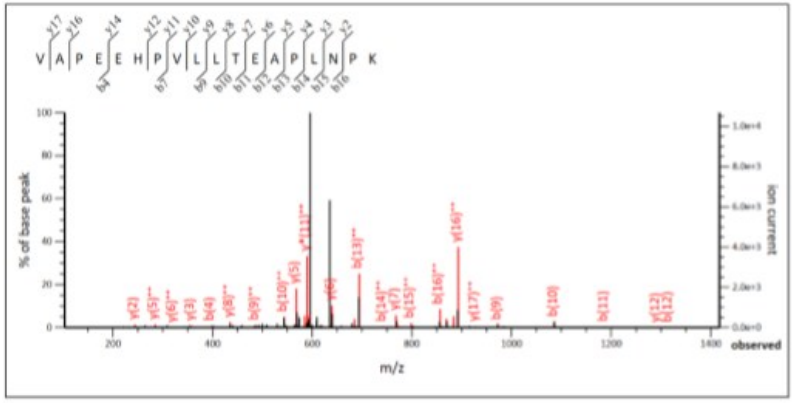
MS/MS Fragmentation of **VAPEEHPVLLTEAPLNPK**

Found in **gi|28252** in **NCBInr_human**, unnamed protein product [Homo sapiens]

Match to Query 1344: 1955.350509 from(652.790894,3+)

Title: spectrumId=1690 Filter=ITMS + c NSI d Full ms2 652.79@cid35.00 [165.00-1320.00] PeakProcessing=continuous Polarity=positive

ScanMode=MassScan TimeInMinutes=12.834872 acqNumber=1690



#	b	b**	b*	b***	b°	b°**	Seq.	y	y**	y*	y***	y°	y°**	#
1	100.1385	50.5729					V							18
2	171.2164	86.1119					A	1856.1033	**928.5553**	1839.0728	920.0401	1838.0880	919.5477	17
3	268.3316	134.6695					P	1785.0254	***893.0164***	1767.9949	884.5011	1767.0101	884.0087	16
4	**397.4456**	199.2265			379.4303	190.2189	E	1687.9102	844.4588	1670.8797	835.9435	1669.8949	835.4511	15
5	526.5596	263.7835			508.5443	254.7759	E	1558.7962	***779.9018***	1541.7657	771.3865	1540.7809	770.8941	14
6	663.6989	332.3531			645.6836	323.3455	H	1429.6822	715.3448	1412.6517	706.8295	1411.6669	706.3371	13
7	760.8141	380.9107			742.7988	371.9031	P	***1292.5429***	646.7751	1275.5124	638.2599	1274.5276	637.7675	12
8	859.9452	430.4763			841.9299	421.4687	V	1195.4277	598.2175	1178.3972	589.7023	1177.4124	589.2099	11
9	**973.1028**	**487.0551**			955.0875	478.0475	L	***1096.2966***	548.6520	1079.2661	540.1367	1078.2813	539.6443	10
10	**1086.2604**	**543.6339**			1068.2451	534.6263	L	***983.1390***	***492.0732***	966.1085	483.5579	965.1237	483.0655	9
11	**1187.3643**	**594.1858**			1169.3490	585.1782	T	***869.9814***	***435.4944***	852.9509	426.9791	851.9661	426.4867	8
12	**1316.4783**	658.7428			1298.4630	649.7352	E	***768.8775***	***384.9424***	751.8470	376.4272	750.8622	375.9348	7
13	1387.5562	**694.2818**			1369.5409	685.2742	A	***639.7615***	320.3854	622.7330	311.8702			6
14	1484.6714	**742.8394**			1466.6561	733.8318	P	***568.6856***	***284.8465***	551.6551	276.3312			5
15	1597.8290	**799.4182**			1579.8137	790.4106	L	471.5704	236.2889	454.5399	227.7736			4
16	1711.9316	**856.4695**	1694.9011	847.9542	1693.9163	847.4619	N	***358.4128***	179.7101	341.3823	171.1948			3
17	1809.0468	905.0271	1792.0163	896.5118	1791.0315	896.0195	P	***244.3102***	122.6588	227.2797	114.1435			2
18							K	147.1950	74.1012	130.1645	65.5859			1

Average mass of neutral peptide Mr(calc): 1954.2269 **Fixed modifications:** Carbamidomethyl (C) (apply to specified residues or termini only) **Ions Score:** 36

Expect: 1.3 **Matches :** 41/156 fragment ions using 102 most intense peaks

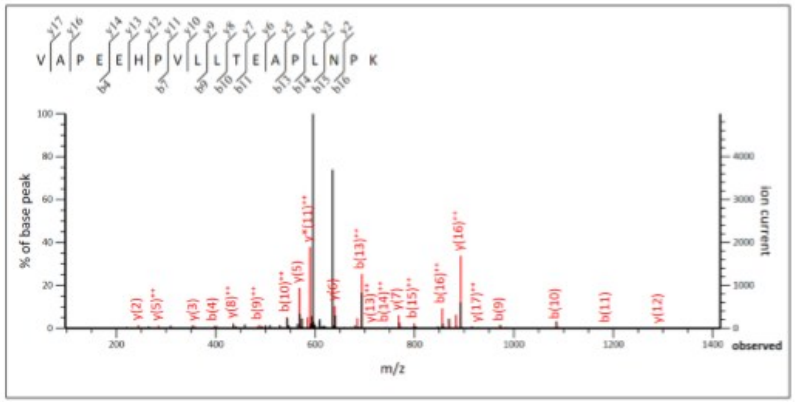
Peptide View

MS/MS Fragmentation of **IKIIAPPER**

Found in **gi|28252** in **NCBInr_human**, unnamed protein product [Homo sapiens]

Match to Query 926: 1036.428090 from(519.221436,2+)

Title: spectrumId=1481 Filter=ITMS + c NSI d Full ms2 519.22@cid35.00 [130.00-1050.00] PeakProcessing=continuous Polarity=positive ScanMode=MassScan TimeInMinutes=10.225383 acqNumber=1481



#	b	b**	b*	b***	b°	b°**	Seq.	y	y**	y*	y***	y°	y°**	#
1	100.1385	50.5729					V							18
2	171.2164	86.1119					A	1856.1033	928.5553	1839.0728	920.0401	1838.0888	919.5477	17
3	268.3316	134.6695					P	1785.0254	893.0164	1767.9949	884.5011	1767.0101	884.0087	16
4	397.4456	199.2265			379.4303	190.2189	E	1687.9107	844.4588	1670.8797	835.9435	1669.8949	835.4511	15
5	526.5596	263.7835			508.5443	254.7759	E	1558.7962	779.9018	1541.7657	771.3865	1540.7809	770.8941	14
6	663.6989	332.3531			645.6836	323.3455	H	1429.6822	715.3448	1412.6517	706.8295	1411.6669	706.3371	13
7	760.8141	380.9107			742.7988	371.9031	P	1292.5429	646.7751	1275.5124	638.2599	1274.5276	637.7675	12
8	859.9452	430.4763			841.9299	421.4687	V	1195.4277	598.2175	1178.3972	589.7023	1177.4124	589.2099	11
9	973.1028	487.0551			955.0875	478.0475	L	1096.2966	548.6520	1079.2661	540.1367	1078.2813	539.6443	10
10	1086.2604	543.6339			1068.2451	534.6263	L	983.1590	492.0732	966.1085	483.5579	965.1237	483.0655	9
11	1187.3643	594.1858			1169.3490	585.1782	T	869.9814	435.4944	852.9509	426.9791	851.9661	426.4867	8
12	1316.4783	658.7428			1298.4630	649.7352	E	768.8775	384.9424	751.8470	376.4272	750.8622	375.9348	7
13	1387.5562	694.2818			1369.5409	685.2742	A	639.7615	320.3844	622.7330	311.8702			6
14	1484.6714	742.8394			1466.6561	733.8318	P	568.6856	284.8465	551.6551	276.3312			5
15	1597.8290	799.4182			1579.8137	790.4106	L	471.5704	236.2889	454.5399	227.7736			4
16	1711.9316	856.4695	1694.9011	847.9542	1693.9163	847.4619	N	358.4128	179.7101	341.3823	171.1948			3
17	1809.0468	905.0271	1792.0163	896.5118	1791.0315	896.0195	P	244.3102	122.6588	227.2797	114.1435			2
18							K	147.1950	74.1012	130.1645	65.5859			1

Average mass of neutral peptide Mr(calc): 1954.2269 **Fixed modifications:** Carbamidomethyl (C) (apply to specified residues or termini only) **Ions Score:** 39 **Expect:** 0.61 **Matches :** 46/156 fragment ions using 109 most intense peaks

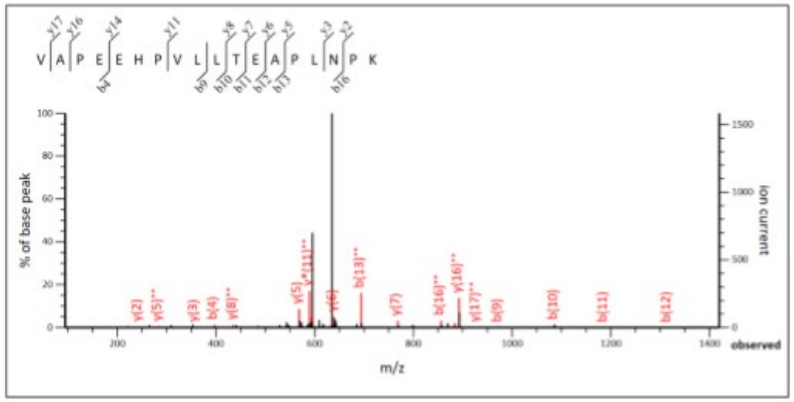
Peptide View

MS/MS Fragmentation of **VAPEEHPVLLTEAPLNPK**

Found in **gi|28252** in **NCBInr_human**, unnamed protein product [Homo sapiens]

Match to Query 1346: 1955.356734 from(652.792969,3+)

Title: spectrumId=1755 Filter=ITMS + c NSI d Full ms2 652.79@cid35.00 [165.00-1320.00] PeakProcessing=continuous Polarity=positive ScanMode=MassScan TimeInMinutes=13.651792 acqNumber=1755



#	b	b**	b*	b***	b°	b°**	Seq.	y	y**	y*	y***	y°	y°**	#
1	100.1385	50.5729					V							18
2	171.2164	86.1119					A	1856.1033	928.5553	1839.0728	920.0401	1838.0880	919.5477	17
3	268.3316	134.6695					P	1785.0254	893.0164	1767.9949	884.5011	1767.0101	884.0087	16
4	397.4456	199.2265			379.4303	190.2189	E	1687.9107	844.4588	1670.8797	835.9435	1669.8949	835.4511	15
5	526.5596	263.7835			508.5443	254.7759	E	1558.7962	779.9018	1541.7657	771.3865	1540.7809	770.8941	14
6	663.6989	332.3531			645.6836	323.3455	H	1429.6822	715.3448	1412.6517	706.8295	1411.6669	706.3371	13
7	760.8141	380.9107			742.7988	371.9031	P	1292.5429	646.7751	1275.5124	638.2599	1274.5276	637.7675	12
8	859.9452	430.4763			841.9299	421.4687	V	1195.4277	598.2175	1178.3972	589.7023	1177.4124	589.2099	11
9	973.1028	487.0551			955.0875	478.0475	L	1096.2966	548.6520	1079.2661	540.1367	1078.2813	539.6443	10
10	1086.2604	543.6339			1068.2451	534.6263	L	983.1590	492.0732	966.1085	483.5579	965.1237	483.0655	9
11	1187.3643	594.1858			1169.3490	585.1782	T	869.9814	435.4944	852.9509	426.9791	851.9661	426.4867	8
12	1316.4783	658.7428			1298.4630	649.7352	E	768.8775	384.9424	751.8470	376.4272	750.8622	375.9348	7
13	1387.5562	694.2818			1369.5409	685.2742	A	639.7615	320.3844	622.7330	311.8702			6
14	1484.6714	742.8394			1466.6561	733.8318	P	568.6856	284.8465	551.6551	276.3312			5
15	1597.8290	799.4182			1579.8137	790.4106	L	471.5704	236.2889	454.5399	227.7736			4
16	1711.9316	856.4695	1694.9011	847.9542	1693.9163	847.4619	N	358.4128	179.7101	341.3823	171.1948			3
17	1809.0468	905.0271	1792.0163	896.5118	1791.0315	896.0195	P	244.3102	122.6588	227.2797	114.1435			2
18							K	147.1950	74.1012	130.1645	65.5859			1

Average mass of neutral peptide Mr(calc): 1954.2269 **Fixed modifications:** Carbamidomethyl (C) (apply to specified residues or termini only) **Ions Score:** 24 **Expect:** 21 **Matches :** 22/156 fragment ions using 44 most intense peaks

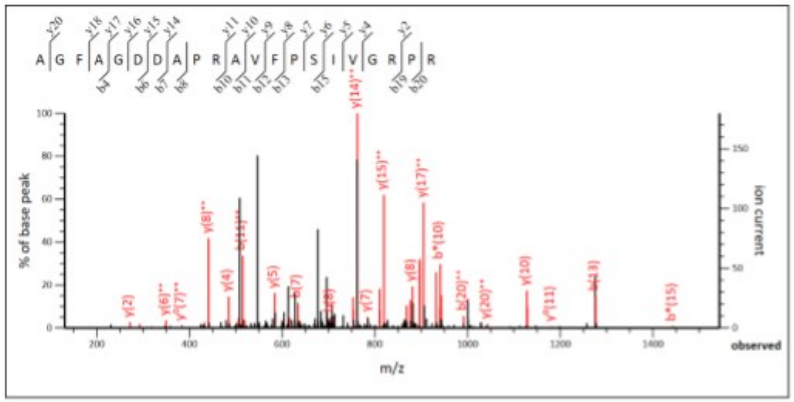
Peptide View

MS/MS Fragmentation of **AGFAGDDAPRAVFPSIVGRPR**

Found in **gi|28252** in **NCBInr_human**, unnamed protein product [Homo sapiens]

Match to Query 1531: 2156.002059 from(719.674744,3+)

Title: spectrumId=1771 Filter=ITMS + c NSI d Full ms2 719.67@cid35.00 [185.00-1450.00] PeakProcessing=continuous Polarity=positive ScanMode=MassScan TimeInMinutes=13.855678 acqNumber=1771



#	b	b++	b*	b*++	b0	b0++	Seq.	y	y++	y*	y*++	y0	y0++	#
1	72.0813	36.5443					A							21
2	129.1366	65.0720					G	2086.5375	1043.6760	2069.5075	1035.1548	2068.5175	1034.6654	20
3	276.3105	138.6589					F	2029.2814	1015.1444	2012.2509	1006.6291	2011.2661	1006.1367	19
4	347.3884	174.1979					A	1882.1075	941.5574	1865.0770	933.0422	1864.0922	932.5498	18
5	404.4397	202.7235					G	1811.0796	906.0435	1793.9991	897.5032	1793.0143	897.0108	17
6	519.5271	260.2672			501.5118	251.2596	D	1753.9783	877.4928	1736.9478	868.9776	1735.9630	868.4852	16
7	634.6145	317.8109			616.5992	308.8033	D	1638.8909	819.9491	1621.8604	811.4339	1620.8756	810.9415	15
8	705.6924	353.3499			687.6771	344.3423	A	1523.8035	762.4054	1506.7730	753.8902	1505.7882	753.3978	14
9	802.8076	401.9075			784.7923	392.8999	P	1452.7256	726.8665	1435.6951	718.3512	1434.7103	717.8588	13
10	958.9933	480.0003	941.9628	471.4851	940.9780	470.9927	R	1355.6104	678.3089	1338.5799	669.7936	1337.5951	669.3012	12
11	1030.0712	515.5393	1013.0407	507.0240	1012.0559	506.5317	A	1199.4741	600.2407	1182.4436	591.7255	1181.4588	591.2334	11
12	1129.2023	565.1048	1112.1718	556.5896	1111.1870	556.0972	V	1128.3163	564.6617	1111.3163	556.1618	1110.3315	555.6694	10
13	1276.3762	638.6918	1259.3457	630.1765	1258.3609	629.6842	F	1029.2157	515.1115	1012.1852	506.5963	1011.2004	506.1039	9
14	1373.4914	687.2494	1356.4609	678.7341	1355.4761	678.2418	P	882.0438	441.5256	865.0133	433.0093	864.0285	432.5169	8
15	1460.5687	730.7880	1443.5382	722.2728	1442.5534	721.7804	S	784.9206	392.9639	767.8961	384.4517	766.9113	383.9593	7
16	1573.7263	787.3668	1556.6958	778.8516	1555.7110	778.3592	I	697.8493	349.4283	680.8188	340.9131			6
17	1672.8374	836.9324	1655.8069	828.4171	1654.8421	827.9248	V	584.6917	292.8495	567.6612	284.3343			5
18	1729.9087	865.4580	1712.8782	856.9428	1711.8934	856.4504	G	485.5606	243.2840	468.5301	234.7687			4
19	1886.0944	943.5509	1869.0639	935.0356	1868.0791	934.5433	R	428.5093	214.7583	411.4788	206.2431			3
20	1983.2096	992.1085	1966.1791	983.5932	1965.1943	983.1009	P	272.1236	136.6655	255.0931	128.1502			2
21							R	175.2084	88.1079	158.1779	79.5926			1

Average mass of neutral peptide Mr(calc): 2156.4032 **Fixed modifications:** Carbamidomethyl (C) (apply to specified residues or termini only) **Ions Score:** 55 **Expect:** 0.011 **Matches :** 48/200 fragment ions using 83 most intense peaks

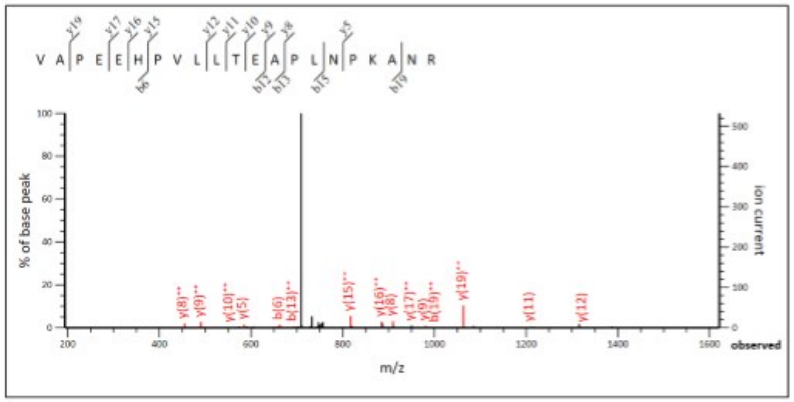
Peptide View

MS/MS Fragmentation of **VAPEEHPVLLTEAPLNPKANR**

Found in **gi|28252** in **NCBInr_human**, unnamed protein product [Homo sapiens]

Match to Query 1596: 2294.828229 from(765.950134,3+)

Title: spectrumId=1631 Filter=ITMS + c NSI d Full ms2 765.95@cid35.00 [200.00-1545.00] PeakProcessing=continuous Polarity=positive ScanMode=MassScan TimeInMinutes=12.094430 acqNumber=1631



#	b	b++	b*	b*++	b0	b0++	Seq.	y	y++	y*	y*++	y0	y0++	#
1	100.1385	50.5729					V							21
2	171.2164	86.1119					A	2197.4695	1099.2384	2180.4390	1090.7232	2179.4542	1090.2308	20
3	268.3316	134.6695					P	2126.9910	1063.6995	2109.9611	1055.1842	2108.9763	1054.6918	19
4	397.4456	199.2265			379.4303	190.2189	E	2029.2764	1015.1419	2012.2459	1006.6266	2011.2611	1006.1342	18
5	526.5596	263.7835			508.5443	254.7759	E	1900.1624	950.5849	1883.1319	942.0696	1882.1471	941.5772	17
6	663.6089	332.3581			645.5936	323.3455	H	1771.0484	886.0279	1754.0179	877.5126	1753.0331	877.0202	16
7	760.8141	380.9107			742.7988	371.9031	P	1633.9091	817.4582	1616.8786	808.9430	1615.8938	808.4506	15
8	859.9452	430.4763			841.9299	421.4687	V	1536.7939	768.9006	1519.7634	760.3854	1518.7786	759.8930	14
9	973.1028	487.0551			955.0875	478.0475	L	1437.6628	719.3351	1420.6323	710.8198	1419.6475	710.3274	13
10	1086.2604	543.6339			1068.2451	534.6263	L	1324.5052	662.7563	1307.4747	654.2410	1306.4899	653.7486	12
11	1187.3641	594.1858			1169.3490	585.1782	T	1211.3476	606.1775	1194.3171	597.6622	1193.3323	597.1698	11
12	1316.4783	658.7428			1298.4630	649.7352	E	1110.2435	555.6254	1093.2130	547.1102	1092.2284	546.6179	10
13	1387.5562	694.2818			1369.5409	685.2742	A	981.1297	491.0685	964.0992	482.5533			9
14	1484.6714	742.8394			1466.6561	733.8318	P	910.0518	455.5296	893.0213	447.0143			8
15	1597.8290	799.4182			1579.8137	790.4106	L	812.9366	406.9720	795.9061	398.4567			7
16	1711.9316	856.4695	1694.9011	847.9542	1693.9163	847.4619	N	699.7790	350.3932	682.7485	341.8779			6
17	1809.0468	905.0271	1792.0163	896.5118	1791.0315	896.0195	P	585.6764	293.3419	568.6459	284.8266			5
18	1937.2191	969.1132	1920.1886	960.5980	1919.2038	960.1056	K	488.5612	244.7843	471.5307	236.2690			4
19	2008.2970	1004.6522	1991.2665	996.1369	1990.2817	995.6446	A	360.3889	180.6981	343.3584	172.1829			3
20	2123.3996	1061.7035	2105.3691	1053.1882	2104.3843	1052.6959	N	289.3518	145.1795	272.2805	136.6439			2
21							R	175.2084	88.1079	158.1779	79.5926			1

Average mass of neutral peptide Mr(calc): 2295.5931 **Fixed modifications:** Carbamidomethyl (C) (apply to specified residues or termini only) **Ions Score:** 20 **Expect:** 46 **Matches :** 20/186 fragment ions using 55 most intense peaks