

Supplementary data for article:

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Electronic Supplementary Material 2

Identification of protein binders in artworks by MALDI-TOF/TOF tandem mass spectrometry

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Electronic Supplementary Material 2 contains MS/MS fragmentation tables related to figures of the manuscript. Fragmentation ion tables are imported from Mascot, while spectra are loaded from BioTools after ion series annotation. Ion series considered during database search were default for MALDI-TOF/TOF in Mascot. Annotations in BioTools were according ion series preset “PSD DeNovo”, similar to the MALDI-TOF/TOF in Mascot, considering a-, b-, b-NH₃ (if R, K, N or Q are included), b-H₂O (if S, T, E or D are included), b+ H₂O, y-, y-NH₃ (if R, K, N or Q are included) ion series, immonium ions and internal fragments.

Details related to Figure 1 of the manuscript

MS/MS Fragmentation of **YLGYLEQLLR**

Found in **CASA1_BOVIN** in SwissProt, Alpha-S1-casein OS=Bos taurus GN=CSN1S1 PE=1 SV=2

Mascot ion score 81 (Individual ions scores > 39 indicate identity or extensive homology (p<0.05)).

#	Immon.	a	a*	a ⁰	b	b*	b ⁰	Seq.	y	y*	y ⁰	#
1	136.0757	136.0757			164.0706			Y				10
2	86.0964	249.1598			277.1547			L	1104.6412	1087.6146	1086.6306	9
3	30.0338	306.1812			334.1761			G	991.5571	974.5306	973.5465	8
4	136.0757	469.2445			497.2395			Y	934.5356	917.5091	916.5251	7
5	86.0964	582.3286			610.3235			L	771.4723	754.4458	753.4617	6
6	102.0550	711.3712		693.3606	739.3661		721.3556	E	658.3883	641.3617	640.3777	5
7	101.0709	839.4298	822.4032	821.4192	867.4247	850.3981	849.4141	Q	529.3457	512.3191		4
8	86.0964	952.5138	935.4873	934.5033	980.5088	963.4822	962.4982	L	401.2871	384.2605		3
9	86.0964	1065.5979	1048.5714	1047.5873	1093.5928	1076.5663	1075.5823	L	288.2030	271.1765		2
10	129.1135							R	175.1190	158.0924		1

RMS error 183 ppm

Details related to Figure 2 a) of the manuscript

MS/MS Fragmentation of **HIATNAVLFFGR** Found in **OVAL_CHICK** in SwissProt, Ovalbumin OS=Gallus gallus

GN=SERPINB14 PE=1 SV=2

Mascot ion score 101 (Individual ions scores > 40 indicate identity or extensive homology (p<0.05)).

#	Immon.	a	a*	a ⁰	b	b*	b ⁰	Seq.	y	y*	y ⁰	#
1	110.0713	110.0713			138.0662			H				12
2	86.0964	223.1553			251.1503			I	1208.6786	1191.6521	1190.6681	11
3	44.0495	294.1925			322.1874			A	1095.5946	1078.5680	1077.5840	10
4	74.0600	395.2401		377.2296	423.2350		405.2245	T	1024.5574	1007.5309	1006.5469	9
5	87.0553	509.2831	492.2565	491.2725	537.2780	520.2514	519.2674	N	923.5098	906.4832		8
6	44.0495	580.3202	563.2936	562.3096	608.3151	591.2885	590.3045	A	809.4668	792.4403		7
7	72.0808	679.3886	662.3620	661.3780	707.3835	690.3570	689.3729	V	738.4297	721.4032		6
8	86.0964	792.4726	775.4461	774.4621	820.4676	803.4410	802.4570	L	639.3613	622.3348		5
9	120.0808	939.5411	922.5145	921.5305	967.5360	950.5094	949.5254	F	526.2772	509.2507		4
10	120.0808	1086.6095	1069.5829	1068.5989	1114.6044	1097.5778	1096.5938	F	379.2088	362.1823		3
11	30.0338	1143.6309	1126.6044	1125.6204	1171.6259	1154.5993	1153.6153	G	232.1404	215.1139		2
12	129.1135							R	175.1190	158.0924		1

RMS error 141 ppm

Details related to Figure 2 b) of the manuscript

MS/MS Fragmentation of **HIATNAVLFFGR**

Found in **OVAL_CHICK** in SwissProt, Ovalbumin OS=Gallus gallus GN=SERPINB14 PE=1 SV=2
 Mascot ion score 75 (Individual ions scores > 40 indicate identity or extensive homology (p<0.05)).

#	Immon.	a	a*	a ⁰	b	b*	b ⁰	Seq.	y	y*	y ⁰	#
1	110.0713	110.0713			138.0662			H				12
2	86.0964	223.1553			251.1503			I	1208.6786	1191.6521	1190.6681	11
3	44.0495	294.1925			322.1874			A	1095.5946	1078.5680	1077.5840	10
4	74.0600	395.2401		377.2296	423.2350		405.2245	T	1024.5574	1007.5309	1006.5469	9
5	87.0553	509.2831	492.2565	491.2725	537.2780	520.2514	519.2674	N	923.5098	906.4832		8
6	44.0495	580.3202	563.2936	562.3096	608.3151	591.2885	590.3045	A	809.4668	792.4403		7
7	72.0808	679.3886	662.3620	661.3780	707.3835	690.3570	689.3729	V	738.4297	721.4032		6
8	86.0964	792.4726	775.4461	774.4621	820.4676	803.4410	802.4570	L	639.3613	622.3348		5
9	120.0808	939.5411	922.5145	921.5305	967.5360	950.5094	949.5254	F	526.2772	509.2507		4
10	120.0808	1086.6095	1069.5829	1068.5989	1114.6044	1097.5778	1096.5938	F	379.2088	362.1823		3
11	30.0338	1143.6309	1126.6044	1125.6204	1171.6259	1154.5993	1153.6153	G	232.1404	215.1139		2
12	129.1135							R	175.1190	158.0924		1

RMS error 341 ppm

Details related to Figure 3 of the manuscript

MS/MS Fragmentation of **FFVAPFPEVFGK**

Found in **CASA1_BOVIN** in SwissProt, Alpha-S1-casein OS=Bos taurus GN=CSN1S1 PE=1 SV=2
 Mascot ion score 70 (Individual ions scores > 39 indicate identity or extensive homology (p<0.05)).

#	Immon.	a	a ⁰	b	b ⁰	Seq.	y	y*	y ⁰	#
1	120.0808	120.0808		148.0757		F				12
2	120.0808	267.1492		295.1441		F	1237.6616	1220.6350	1219.6510	11
3	72.0808	366.2176		394.2125		V	1090.5932	1073.5666	1072.5826	10
4	44.0495	437.2547		465.2496		A	991.5247	974.4982	973.5142	9
5	70.0651	534.3075		562.3024		P	920.4876	903.4611	902.4771	8
6	120.0808	681.3759		709.3708		F	823.4349	806.4083	805.4243	7
7	70.0651	778.4287		806.4236		P	676.3665	659.3399	658.3559	6
8	102.0550	907.4713	889.4607	935.4662	917.4556	E	579.3137	562.2871	561.3031	5
9	72.0808	1006.5397	988.5291	1034.5346	1016.5240	V	450.2711	433.2445		4
10	120.0808	1153.6081	1135.5975	1181.6030	1163.5924	F	351.2027	334.1761		3
11	30.0338	1210.6295	1192.6190	1238.6245	1220.6139	G	204.1343	187.1077		2
12	101.1073					K	147.1128	130.0863		1

RMS error 255 ppm

Details related to Figure 4 of the manuscript

MS/MS Fragmentation of **GIPGEFGLPGPAGAR 3: Oxidation (P) 9: Oxidation (P)**

Found in **CO1A2_BOVIN** in SwissProt, Collagen alpha-2(I) chain OS=Bos taurus GN=COL1A2 PE=1 SV=2
 Mascot ion score 70 (Individual ions scores > 38 indicate identity or extensive homology (p<0.05)).

#	Immon.	a	a ⁰	b	b ⁰	Seq.	y	y*	y ⁰	#
1	30.0338	30.0338		58.0287		G				15
2	86.0964	143.1179		171.1128		I	1370.7063	1353.6797	1352.6957	14
3	86.0600	256.1656		284.1605		P	1257.6222	1240.5957	1239.6117	13
4	30.0338	313.1870		341.1819		G	1144.5746	1127.5480	1126.5640	12
5	102.0550	442.2296	424.2191	470.2245	452.2140	E	1087.5531	1070.5265	1069.5425	11
6	120.0808	589.2980	571.2875	617.2930	599.2824	F	958.5105	941.4839		10
7	30.0338	646.3195	628.3089	674.3144	656.3039	G	811.4421	794.4155		9
8	86.0964	759.4036	741.3930	787.3985	769.3879	L	754.4206	737.3941		8
9	86.0600	872.4512	854.4407	900.4462	882.4356	P	641.3366	624.3100		7
10	30.0338	929.4727	911.4621	957.4676	939.4571	G	528.2889	511.2623		6
11	70.0651	1026.5255	1008.5149	1054.5204	1036.5098	P	471.2674	454.2409		5
12	44.0495	1097.5626	1079.5520	1125.5575	1107.5469	A	374.2146	357.1881		4
13	30.0338	1154.5841	1136.5735	1182.5790	1164.5684	G	303.1775	286.1510		3
14	44.0495	1225.6212	1207.6106	1253.6161	1235.6055	A	246.1561	229.1295		2
15	129.1135					R	175.1190	158.0924		1

RMS error 268 ppm

Details related to Figure 6 of the manuscript

MS/MS Fragmentation of **GIPGEFGLPGPAGAR 3: Oxidation (P) 9: Oxidation (P)**

Found in **CO1A2_BOVIN** in SwissProt, Collagen alpha-2(I) chain OS=Bos taurus GN=COL1A2 PE=1 SV=2
 Mascot ion score 19 (Individual ions scores > 36 indicate identity or extensive homology (p<0.05)).

#	Immon.	a	a ⁰	b	b ⁰	Seq.	y	y*	y ⁰	#
1	30.0338	30.0338		58.0287		G				15
2	86.0964	143.1179		171.1128		I	1370.7063	1353.6797	1352.6957	14
3	86.0600	256.1656		284.1605		P	1257.6222	1240.5957	1239.6117	13
4	30.0338	313.1870		341.1819		G	1144.5746	1127.5480	1126.5640	12
5	102.0550	442.2296	424.2191	470.2245	452.2140	E	1087.5531	1070.5265	1069.5425	11
6	120.0808	589.2980	571.2875	617.2930	599.2824	F	958.5105	941.4839		10
7	30.0338	646.3195	628.3089	674.3144	656.3039	G	811.4421	794.4155		9
8	86.0964	759.4036	741.3930	787.3985	769.3879	L	754.4206	737.3941		8
9	86.0600	872.4512	854.4407	900.4462	882.4356	P	641.3366	624.3100		7
10	30.0338	929.4727	911.4621	957.4676	939.4571	G	528.2889	511.2623		6
11	70.0651	1026.5255	1008.5149	1054.5204	1036.5098	P	471.2674	454.2409		5
12	44.0495	1097.5626	1079.5520	1125.5575	1107.5469	A	374.2146	357.1881		4
13	30.0338	1154.5841	1136.5735	1182.5790	1164.5684	G	303.1775	286.1510		3
14	44.0495	1225.6212	1207.6106	1253.6161	1235.6055	A	246.1561	229.1295		2
15	129.1135					R	175.1190	158.0924		1

RMS error 1170 ppm