

Supporting Information for

Identification of a Common Recognition Center for a Photoactive Non-steroidal Antiinflammatory Drug in Serum Albumins of Different Species

Oscar Molins-Molina,^[a] Emilio Lence,^[b] Daniel Limones-Herrero,^[a] Concepción González-Bello,^[b] Miguel A. Miranda*^[a] and M. Consuelo Jiménez*^[a]

Page S1- This page.

Page S2- **Figure S1.** Absorption spectra of **CPF**, **SA**, **CPF@SA** and **CPF+SA**.

Pages S3-S29- Amino acid sequence of the different SAs with the altered amino acid residues indicated in red, together with the ESI-MS/MS spectra and fragmentation pathway of each modified peptide. The amino acid number is the one used in the available crystallographic structures where the position of the first 24 amino acids is not resolved

HSA: Pages S3-S5

BSA: Pages S6-S10

PSA: Pages S11-S12

RbSA: Pages S13-S17

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Pages S29- **Figure S2.** Multiple sequence alignment.

Page S30- **Figure S3.** rmsd plots for the three domains protein backbone and ligand calculated for the binary **CPF/HSA-V** cleft complex.

Page S31- **Figure S4.** rmsd plots for the three domains protein backbone (Ca, C, N and O atoms) and ligand calculated for the binary **CPF/HSA-IB** complex.

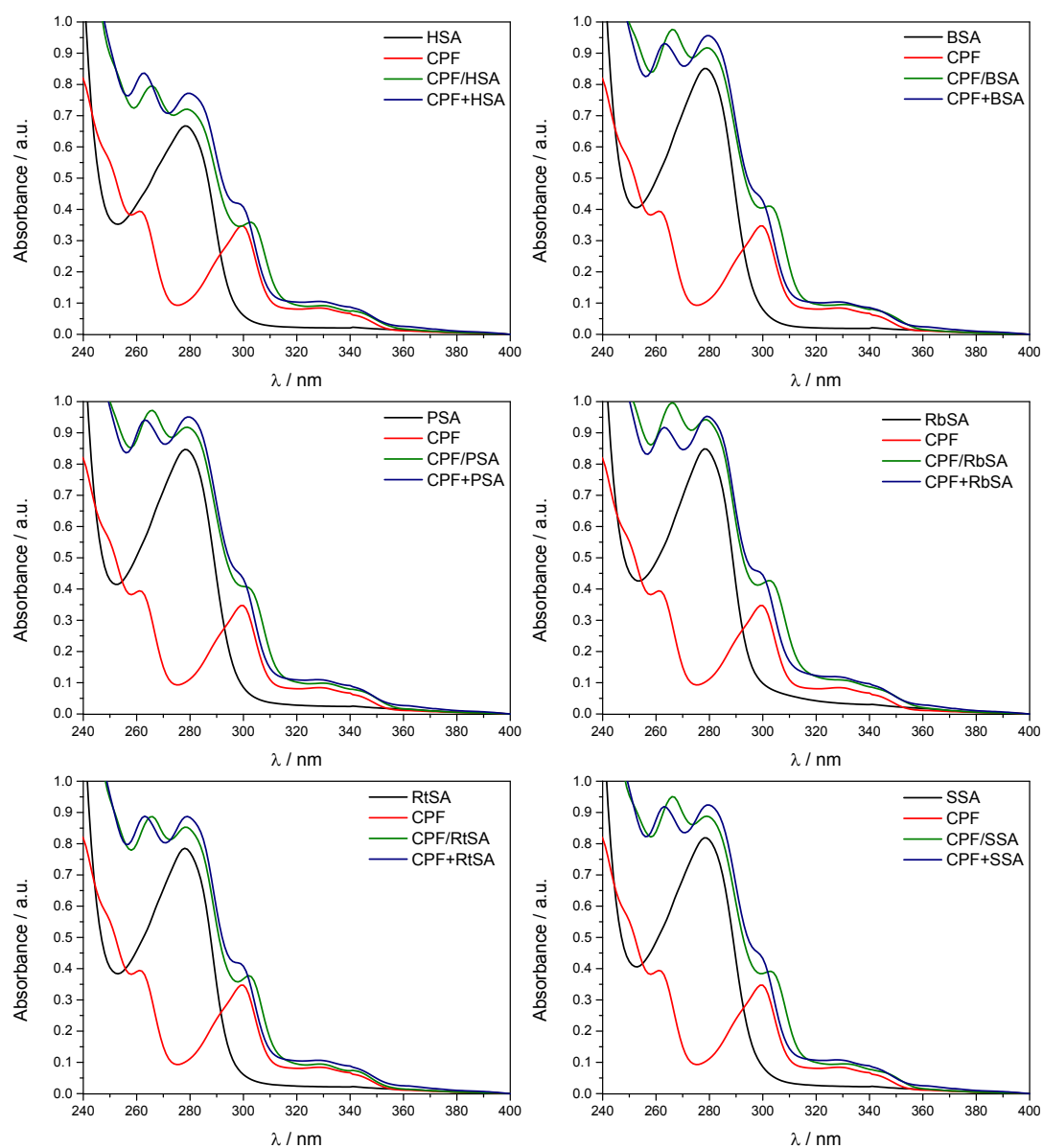


Figure S1. Absorption spectra of **CPF**, **SA**, **CPF/SA** at 1:1 molar ratio and simulated spectra obtained by addition of isolated **CPF** and **SA** spectra (**CPF+SA**). Concentration of drug and protein was 2×10^{-5} M.

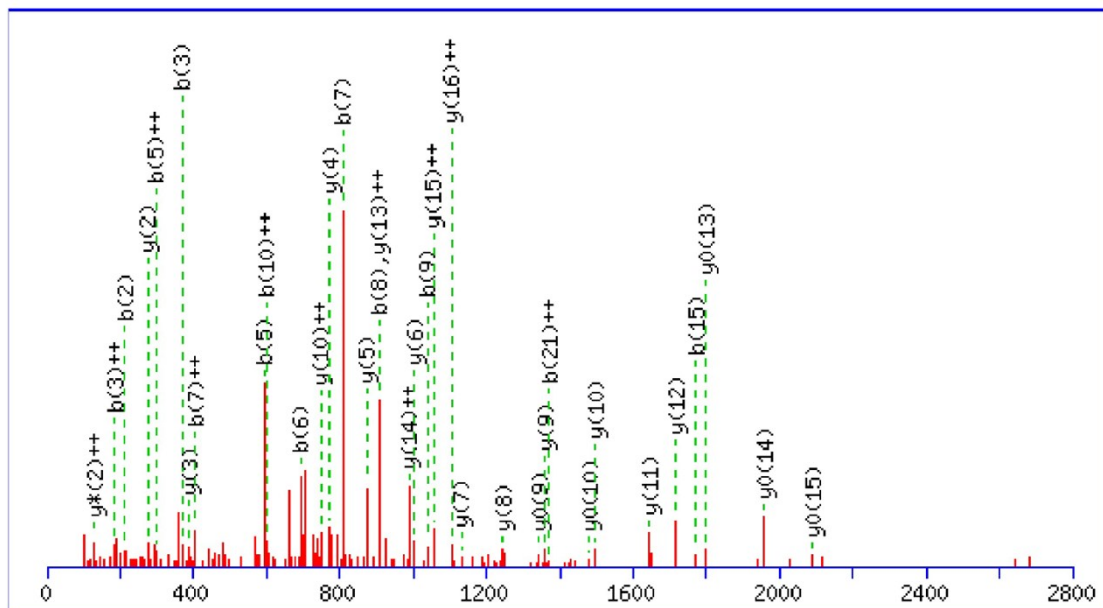
Amino acid sequence of HSA with the altered amino acid residues indicated in red, together with the ESI-MS/MS spectra and fragmentation pathway of each modified peptide

CPF/HSA

1	MKWVTFISLL	FLFSSAYSRG	VFRRDAHKSE	VAHRFKDLGE	ENFKALVLIA
51	FAQYLQQCPF	EDHVKLVNEV	TEFAKTCVAD	ESAENCCKSL	HTLFGDKLCT
101	VATLRETYGE	MADCCAKQEP	ERNECFLOHK	DDNPNLPRLV	RPEVDVMCTA
151	FHDNEETLKK	KYLYEIAARR	PYFYAPELLF	FAKRYKAAFT	ECCQAADKAA
201	CLLPKLDELRL	DEGKASSAKQ	RLKCASLQKF	GERAFKANAV	ARLSQRFPKA
251	EFAEVSKLVT	DLTKVHTECC	HGDLLECADD	RADLAKYICE	NQDSISSKLK
301	ECCEKPLLEK	SHCIAEVEND	EMPADLPSLA	ADFVESKDVC	KNYAEAKDVF
351	LGMFLYEYAR	RHPDYSVLL	LRLAKTYETT	LEKCCAAADP	HECYAKVFDE
401	FKPLVEEPQN	LIKQNCLEFE	QLGEYKFQNA	LLVRYTKKVP	QVSTPTLVEV
451	SRNLGKVGSK	CCKHPEAKRM	PCAEDLSVV	LNQLCVLHEK	TPVSDRVTKC
501	CTESLVNRRP	CFSALEVDET	YVPKEFNAET	FTFHADICTL	SEKERQIKKQ
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601	AASQAALGL				

Phe134

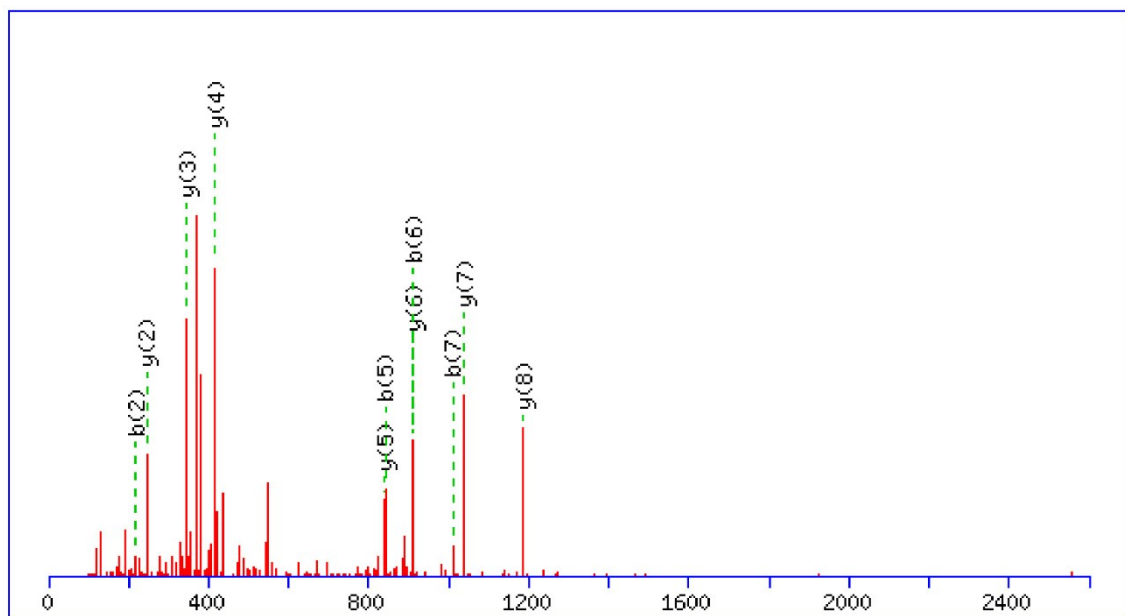
LVRPEVDVMCTAFHDNEETLKK



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1	114.0913	57.5493					L							23
2	213.1598	107.0835					V	2902.3539	1451.6806	2885.3273	1443.1673	2884.3433	1442.6753	22
3	369.2609	185.1341	352.2343	176.6208			R	2803.2855	1402.1464	2786.2589	1393.6331	2785.2749	1393.1411	21
4	466.3136	233.6605	449.2871	225.1472			P	2647.1843	1324.0958	2630.1578	1315.5825	2629.1738	1315.0905	20
5	595.3562	298.1817	578.3297	289.6685	577.3457	289.1765	E	2550.1316	1275.5694	2533.1050	1267.0562	2532.1210	1266.5641	19
6	694.4246	347.7160	677.3981	339.2027	676.4141	338.7107	V	2421.0890	1211.0481	2404.0624	1202.5349	2403.0784	1202.0428	18
7	809.4516	405.2294	792.4250	396.7162	791.4410	396.2241	D	2322.0206	1161.5139	2304.9940	1153.0006	2304.0100	1152.5086	17
8	908.5200	454.7636	891.4934	446.2504	890.5094	445.7584	V	2206.9936	1104.0005	2189.9671	1095.4872	2188.9831	1094.9952	16
9	1039.5605	520.2839	1022.5339	511.7706	1021.5499	511.2786	M	2107.9252	1054.4662	2090.8987	1045.9530	2089.9146	1045.4610	15
10	1199.5911	600.2992	1182.5646	591.7859	1181.5806	591.2939	C	1976.8847	988.9460	1959.8582	980.4327	1958.8742	979.9407	14
11	1300.6388	650.8230	1283.6123	642.3098	1282.6282	641.8178	T	1816.8541	908.9307	1799.8275	900.4174	1798.8435	899.9254	13
12	1371.6759	686.3416	1354.6494	677.8283	1353.6654	677.3363	A	1715.8064	858.4068	1698.7798	849.8936	1697.7958	849.4016	12
13	1518.7443	759.8758	1501.7178	751.3625	1500.7338	750.8705	F	1644.7693	822.8883	1627.7427	814.3750	1626.7587	813.8830	11
14	1655.8032	828.4053	1638.7767	819.8920	1637.7927	819.4000	H	1497.7009	749.3541	1480.6743	740.8408	1479.6903	740.3488	10
15	1770.8302	885.9187	1753.8036	877.4055	1752.8196	876.9135	D	1360.6420	680.8246	1343.6154	672.3113	1342.6314	671.8193	9
16	1884.8731	942.9402	1867.8466	934.4269	1866.8626	933.9349	N	1245.6150	623.3111	1228.5885	614.7979	1227.6045	614.3059	8
17	2013.9157	1007.4615	1996.8892	998.9482	1995.9051	998.4562	E	1131.5721	566.2897	1114.5455	557.7764	1113.5615	557.2844	7
18	2142.9583	1071.9828	2125.9318	1063.4695	2124.9477	1062.9775	E	1002.5295	501.7684	985.5029	493.2551	984.5189	492.7631	6
19	2244.0060	1122.5066	2226.9794	1113.9934	2225.9954	1113.5013	T	873.4869	437.2471	856.4604	428.7338	855.4763	428.2418	5
20	2628.1534	1314.5803	2611.1268	1306.0671	2610.1428	1305.5750	F	772.4392	386.7233	755.4127	378.2100			4
21	2741.2374	1371.1224	2724.2109	1362.6091	2723.2269	1362.1171	L	388.2918	194.6496	371.2653	186.1363			3
22	2869.3324	1435.1698	2852.3059	1426.6566	2851.3218	1426.1646	K	275.2078	138.1075	258.1812	129.5942			2
23							K	147.1128	74.0600	130.0863	65.5468			1

Trp 214

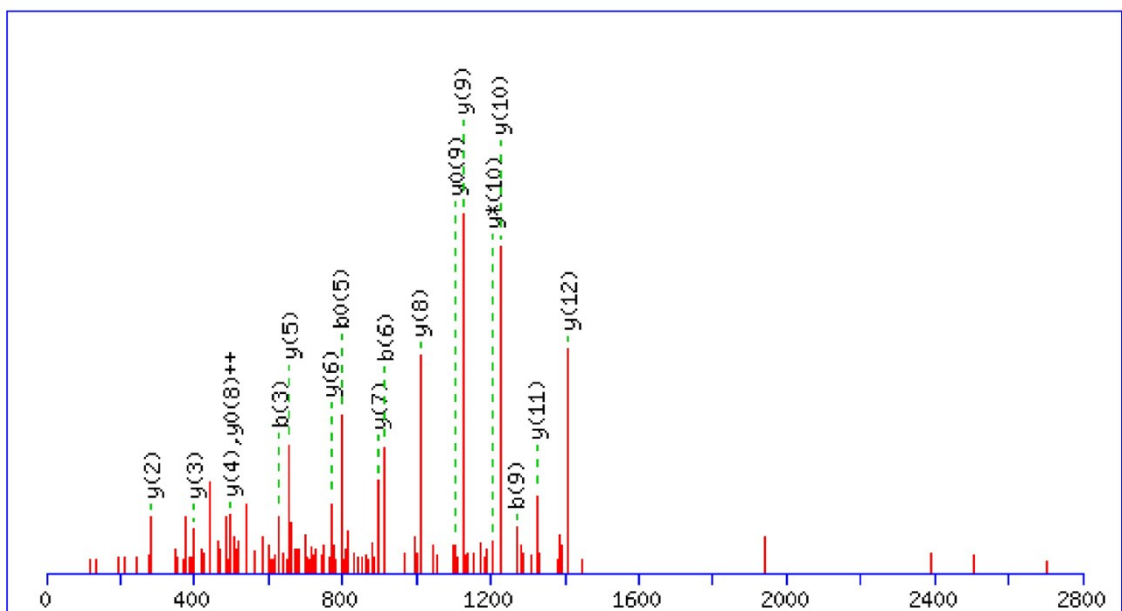
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4	418.2449	209.6261	401.2183	201.1128	A	910.4570	455.7321	893.4305	447.2189	6
5	841.4032	421.2052	824.3766	412.6920	W	839.4199	420.2136	822.3933	411.7003	5
6	912.4403	456.7238	895.4137	448.2105	A	416.2616	208.6344	399.2350	200.1212	4
7	1011.5087	506.2580	994.4822	497.7447	V	345.2245	173.1159	328.1979	164.6026	3
8	1082.5458	541.7765	1065.5193	533.2633	A	246.1561	123.5817	229.1295	115.0684	2
9					R	175.1190	88.0631	158.0924	79.5498	1

Tyr 452

DYLSVVLNQLCVLHE



#	b	b ⁺⁺	b [*]	b ^{*++}	b ⁰	b ⁰⁺⁺	Seq.	y	y ⁺⁺	y [*]	y ^{*++}	y ⁰	y ⁰⁺⁺	#
1	116.0342	58.5207			98.0237	49.5155	D							15
2	516.1765	258.5919			498.1660	249.5866	Y	1923.9673	962.4873	1906.9408	953.9740	1905.9568	953.4820	14
3	629.2606	315.1339			611.2500	306.1287	L	1523.8250	762.4162	1506.7985	753.9029	1505.8145	753.4109	13
4	716.2926	358.6499			698.2821	349.6447	S	1410.7410	705.8741	1393.7144	697.3608	1392.7304	696.8688	12
5	815.3610	408.1842			797.3505	399.1789	V	1323.7089	662.3581	1306.6824	653.8448	1305.6984	653.3528	11
6	914.4294	457.7184			896.4189	448.7131	V	1224.6405	612.8239	1207.6140	604.3106	1206.6300	603.8186	10
7	1027.5135	514.2604			1009.5029	505.2551	L	1125.5721	563.2897	1108.5456	554.7764	1107.5615	554.2844	9
8	1141.5564	571.2819	1124.5299	562.7686	1123.5459	562.2766	N	1012.4880	506.7477	995.4615	498.2344	994.4775	497.7424	8
9	1269.6150	635.3111	1252.5885	626.7979	1251.6045	626.3059	Q	898.4451	449.7262	881.4186	441.2129	880.4346	440.7209	7
10	1382.6991	691.8532	1365.6725	683.3399	1364.6885	682.8479	L	770.3865	385.6969			752.3760	376.6916	6
11	1542.7297	771.8685	1525.7032	763.3552	1524.7192	762.8632	C	657.3025	329.1549			639.2919	320.1496	5
12	1641.7981	821.4027	1624.7716	812.8894	1623.7876	812.3974	V	497.2718	249.1396			479.2613	240.1343	4
13	1754.8822	877.9447	1737.8557	869.4315	1736.8716	868.9395	L	398.2034	199.6053			380.1928	190.6001	3
14	1891.9411	946.4742	1874.9146	937.9609	1873.9306	937.4689	H	285.1193	143.0633			267.1088	134.0580	2
15							E	148.0604	74.5339			130.0499	65.5286	1

Amino acid sequence of BSA with the altered amino acid residues indicated in red, together with the ESI-MS/MS spectra and fragmentation pathway of each modified peptide

CPF/BSA

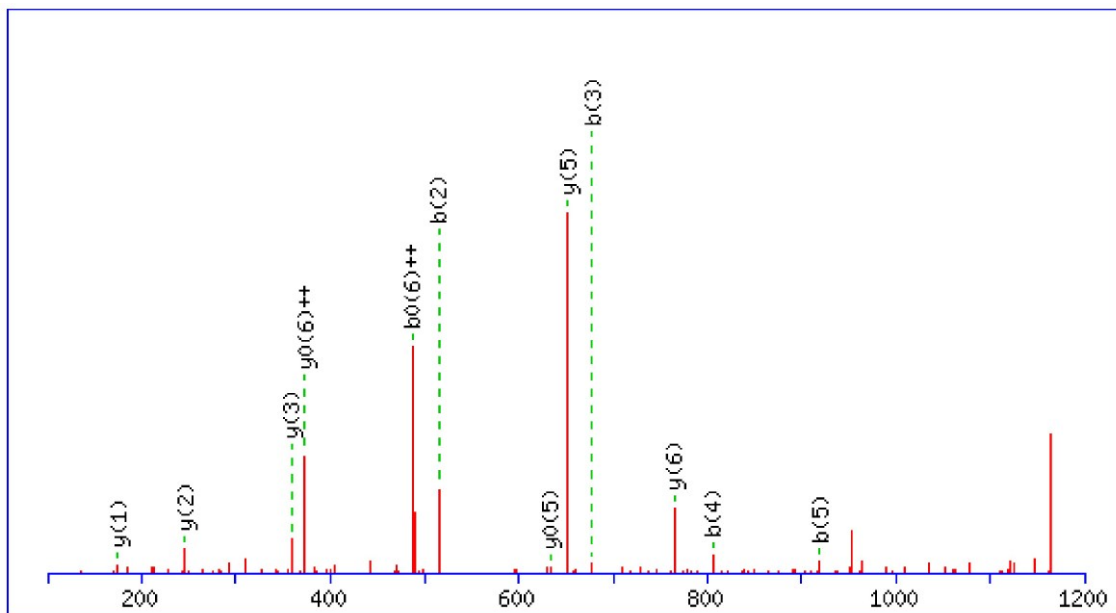
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1  MKWVTFISLL LLFSSAYSRG VFRDTHKSE IAHRFKDLGE EHFKGLVLIA
51  FSQYLQQCPF DEHVKLVELL TEFATCVAD ESHAGCEKSL HTLFGDELCK
101 VASLRETYGD MADCCEKQEP ERNECFLSHK DDSPDLPKLK PDPNTLCDEF
151 KADEKKFWGK YLYEIARRHP YFYAPELLYY ANKYNGVFQE CCQAEDKGAC
201 LLPKIETMRE KVLASSARQR LRCASIQKFG ERALKAWSVA RLSQKFPKAE
251 FVEVTKLVTD LTKVHKECCH GDLLECADDR ADLAKYICDN QDTISSKLKE
301 CCDKPLLEKS HCIAEVEKDA IPENLPPLTA DFAEDKDVCK NYQEAKDAFL
351 GSYLYEYSRR HPEYAVSVLL RLAKEYEATL EECCAADDPH ACYSTVFDFKL
401 KHLVDEPQNL IKQNCQDFEK LGEYGFQNAL IVRYTRKVPQ VSTPTLVEVS
451 RSLGKVGTRC CTKPESERMP CTEDYLSLIL NRCLVLHEKT PVSEKVTKCC
501 TESLVNRRPC FSALTPDETY VPKAFDEKLF TEHADICTLP DTEKQIKKQT
551 ALVELLKHKP KATEEQLKTV MENFVAFVDK CCAADDKEAC FAVEGPKLVV
601 STQTALA

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Tyr137

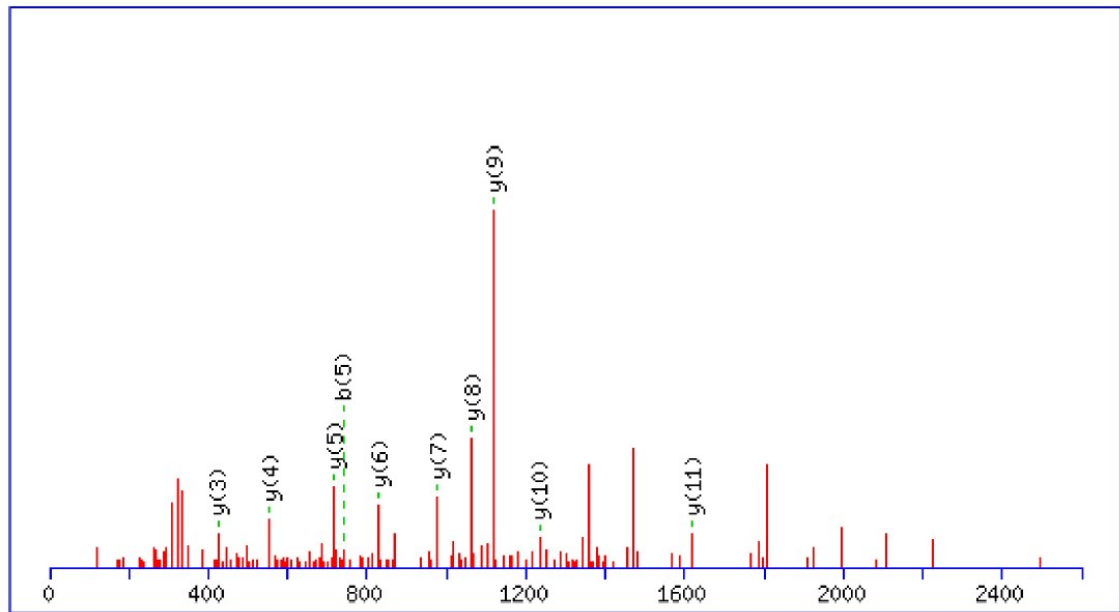
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1	401.1496	201.0784			Y							7
2	514.2336	257.6205			L	764.4301	382.7187	747.4036	374.2054	746.4196	373.7134	6
3	677.2970	339.1521			Y	651.3461	326.1767	634.3195	317.6634	633.3355	317.1714	5
4	806.3396	403.6734	788.3290	394.6681	E	488.2827	244.6450	471.2562	236.1317	470.2722	235.6397	4
5	919.4236	460.2155	901.4131	451.2102	I	359.2401	180.1237	342.2136	171.6104			3
6	990.4607	495.7340	972.4502	486.7287	A	246.1561	123.5817	229.1295	115.0684			2
7					R	175.1190	88.0631	158.0924	79.5498			1

Phe325

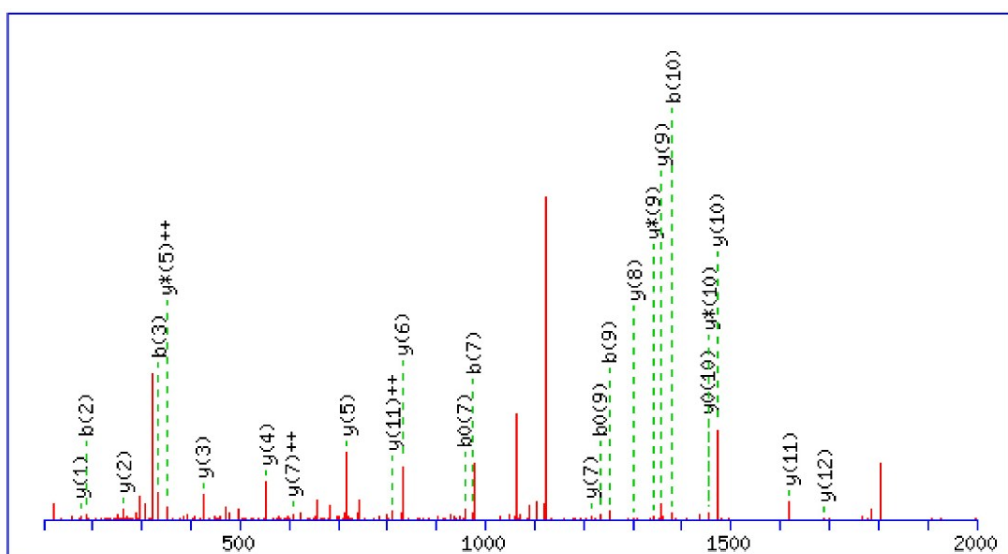
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1	116.0342	58.5207	98.0237	49.5155	D							13
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3	571.2187	286.1130	553.2082	277.1077	F	1618.7577	809.8825	1601.7311	801.3692	1600.7471	800.8772	11
4	684.3028	342.6550	666.2922	333.6498	L	1234.6103	617.8088	1217.5837	609.2955	1216.5997	608.8035	10
5	741.3243	371.1658	723.3137	362.1605	G	1121.5262	561.2667	1104.4997	552.7535	1103.5156	552.2615	9
6	828.3563	414.6818	810.3457	405.6765	S	1064.5047	532.7560	1047.4782	524.2427	1046.4942	523.7507	8
7	975.4247	488.2160	957.4141	479.2107	F	977.4727	489.2400	960.4462	480.7267	959.4621	480.2347	7
8	1088.5088	544.7580	1070.4982	535.7527	L	830.4043	415.7058	813.3777	407.1925	812.3937	406.7005	6
9	1251.5721	626.2897	1233.5615	617.2844	Y	717.3202	359.1638	700.2937	350.6505	699.3097	350.1585	5
10	1380.6147	690.8110	1362.6041	681.8057	E	554.2569	277.6321	537.2304	269.1188	536.2463	268.6268	4
11	1543.6780	772.3426	1525.6674	763.3374	Y	425.2143	213.1108	408.1878	204.5975	407.2037	204.1055	3
12	1630.7100	815.8587	1612.6995	806.8534	S	262.1510	131.5791	245.1244	123.0659	244.1404	122.5738	2
13					R	175.1190	88.0631	158.0924	79.5498			1

Phe329

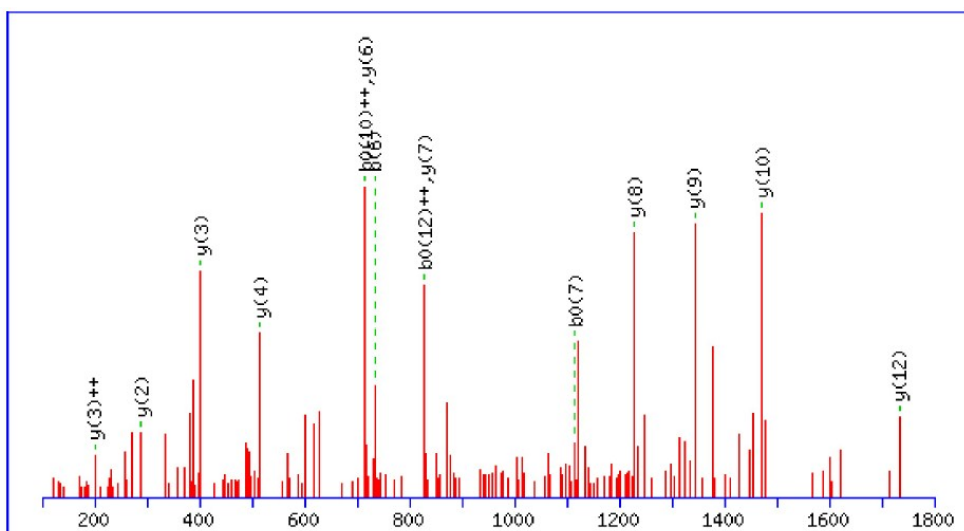
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1	116.0342	58.5207	98.0237	49.5155	D							13
2	187.0713	94.0393	169.0608	85.0340	A	1689.7948	845.4010	1672.7682	836.8877	1671.7842	836.3957	12
3	334.1397	167.5735	316.1292	158.5682	F	1618.7577	809.8825	1601.7311	801.3692	1600.7471	800.8772	11
4	447.2238	224.1155	429.2132	215.1103	L	1471.6892	736.3483	1454.6627	727.8350	1453.6787	727.3430	10
5	504.2453	252.6263	486.2347	243.6210	G	1358.6052	679.8062	1341.5786	671.2930	1340.5946	670.8009	9
6	591.2773	296.1423	573.2667	287.1370	S	1301.5837	651.2955	1284.5572	642.7822	1283.5732	642.2902	8
7	975.4247	488.2160	957.4141	479.2107	F	1214.5517	607.7795	1197.5251	599.2662	1196.5411	598.7742	7
8	1088.5088	544.7580	1070.4982	535.7527	L	830.4043	415.7058	813.3777	407.1925	812.3937	406.7005	6
9	1251.5721	626.2897	1233.5615	617.2844	Y	717.3202	359.1638	700.2937	350.6505	699.3097	350.1585	5
10	1380.6147	690.8110	1362.6041	681.8057	E	554.2569	277.6321	537.2304	269.1188	536.2463	268.6268	4
11	1543.6780	772.3426	1525.6674	763.3374	Y	425.2143	213.1108	408.1878	204.5975	407.2037	204.1055	3
12	1630.7100	815.8587	1612.6995	806.8534	S	262.1510	131.5791	245.1244	123.0659	244.1404	122.5738	2
13					R	175.1190	88.0631	158.0924	79.5498			1

Tyr 451

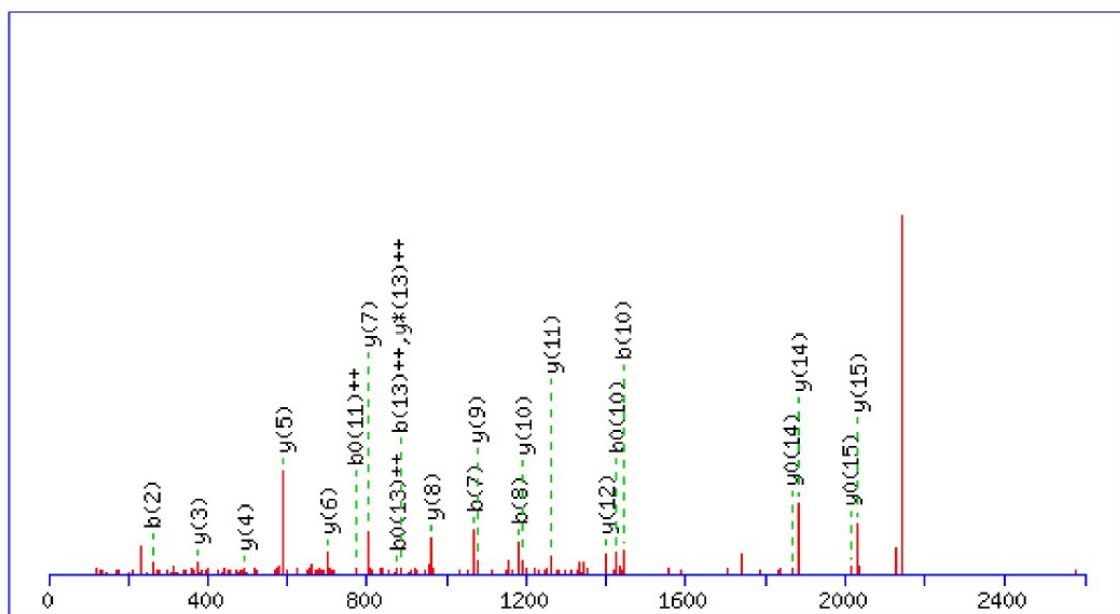
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3	389.1312	195.0692					C	1733.8203	867.4138	1716.7938	858.9005	1715.8098	858.4085	12
4	490.1789	245.5931			472.1683	236.5878	T	1573.7897	787.3985	1556.7631	778.8852	1555.7791	778.3932	11
5	619.2214	310.1144			601.2109	301.1091	E	1472.7420	736.8746	1455.7155	728.3614	1454.7314	727.8694	10
6	734.2484	367.6278			716.2378	358.6225	D	1343.6994	672.3533	1326.6729	663.8401	1325.6888	663.3481	9
7	1134.3907	567.6990			1116.3801	558.6937	Y	1228.6725	614.8399	1211.6459	606.3266	1210.6619	605.8346	8
8	1247.4748	624.2410			1229.4642	615.2357	L	828.5302	414.7687	811.5036	406.2554	810.5196	405.7634	7
9	1334.5068	667.7570			1316.4962	658.7518	S	715.4461	358.2267	698.4195	349.7134	697.4355	349.2214	6
10	1447.5909	724.2991			1429.5803	715.2938	L	628.4141	314.7107	611.3875	306.1974			5
11	1560.6749	780.8411			1542.6644	771.8358	I	515.3300	258.1686	498.3035	249.6554			4
12	1673.7590	837.3831			1655.7484	828.3778	L	402.2459	201.6266	385.2194	193.1133			3
13	1787.8019	894.4046	1770.7754	885.8913	1769.7913	885.3993	N	289.1619	145.0846	272.1353	136.5713			2
14							R	175.1190	88.0631	158.0924	79.5498			1

Phe 508

LFTADICTLPDTEK



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2	261.1598	131.0835			F	2031.9157	1016.4615	2014.8891	1007.9482	2013.9051	1007.4562	15
3	362.2074	181.6074	344.1969	172.6021	T	1884.8473	942.9273	1867.8207	934.4140	1866.8367	933.9220	14
4	746.3548	373.6811	728.3443	364.6758	F	1783.7996	892.4034	1766.7731	883.8902	1765.7890	883.3982	13
5	883.4137	442.2105	865.4032	433.2052	H	1399.6522	700.3297	1382.6257	691.8165	1381.6416	691.3245	12
6	954.4509	477.7291	936.4403	468.7238	A	1262.5933	631.8003	1245.5667	623.2870	1244.5827	622.7950	11
7	1069.4778	535.2425	1051.4672	526.2373	D	1191.5562	596.2817	1174.5296	587.7685	1173.5456	587.2764	10
8	1182.5619	591.7846	1164.5513	582.7793	I	1076.5292	538.7683	1059.5027	530.2550	1058.5187	529.7630	9
9	1342.5925	671.7999	1324.5819	662.7946	C	963.4452	482.2262	946.4186	473.7130	945.4346	473.2209	8
10	1443.6402	722.3237	1425.6296	713.3184	T	803.4145	402.2109	786.3880	393.6976	785.4040	393.2056	7
11	1556.7243	778.8658	1538.7137	769.8605	L	702.3668	351.6871	685.3403	343.1738	684.3563	342.6818	6
12	1653.7770	827.3921	1635.7664	818.3869	P	589.2828	295.1450	572.2562	286.6318	571.2722	286.1397	5
13	1768.8040	884.9056	1750.7934	875.9003	D	492.2300	246.6186	475.2035	238.1054	474.2195	237.6134	4
14	1869.8516	935.4295	1851.8411	926.4242	T	377.2031	189.1052	360.1765	180.5919	359.1925	180.0999	3
15	1998.8942	999.9508	1980.8837	990.9455	E	276.1554	138.5813	259.1288	130.0681	258.1448	129.5761	2
16					K	147.1128	74.0600	130.0863	65.5468			1

Amino acid sequence of PSA with the altered amino acid residues indicated in red, together with the ESI-MS/MS spectra and fragmentation pathway of each modified peptide

CPF/PSA

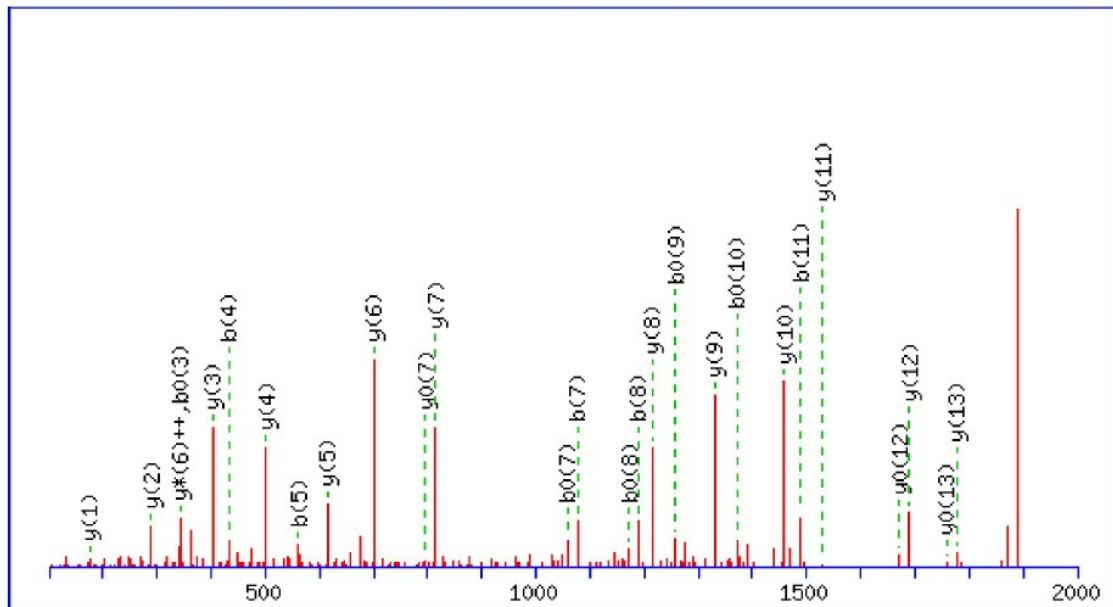
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1  MKWVTFISLL FLFSSAYSRG VFRRDTYKSE IAHRFKDLGE QYFKGLVLIA
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101 IPSLREHYGD LADCCEKEEP ERNECFLQHK NDNPDIPKLK PDPVALCADF
151 QEDEQKFWGK YLYEIARRHP YFYAPELLYY AIIYKDVFSE CCQAADKAAC
201 LLPKIEHLRE KVLTSAAKQR LKASIQKFG ERAFKAWSLA RLSQRFPKAD
251 FTEISKIVTD LAKVHKECCH GDLLCADDR ADLAKYICEN QDTISTKLKE
301 CCDKPLLEKS HCIAEAKRDE LPADLNPLEH DFVEDKEVCK NYKEAKHVFL
351 GTFLYEYSRR HPDYSVSLLL RIAKIYEATL EDCCAKEDPP ACYATVFDKF
401 QPLVDEPKNL IKQNCSELF EK LGEYGFQNAL IVRYTKKVPQ VSTPTLVEVA
451 RKLGLVGSRK CKRPEEERLS CAEDYLSLVL NRLCVLHEKT PVSEKVTKCC
501 TESLVNRRPC FSALTPDETY KPKEFVEGTF TFHADLCTLP EDEKQIKKQT
551 ALVELLKHKP HATEEQLRTV LGNFAAFVQK CCAAPDHEAC FAVEGPKFVI
601 EIRGILA

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Tyr 451

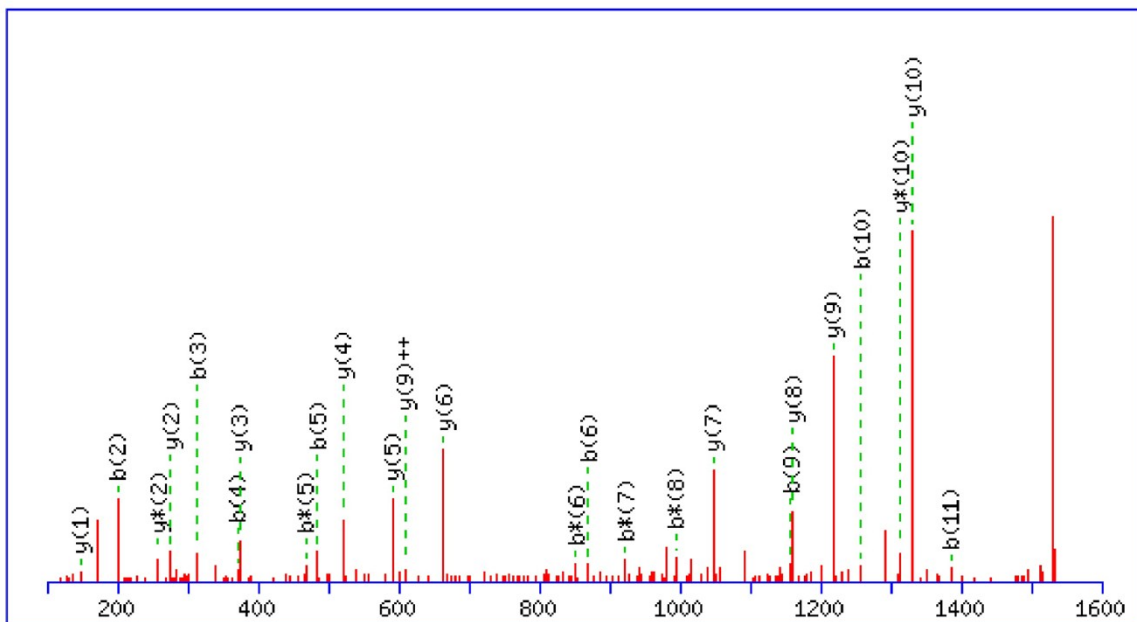
LSCAEDYLSLVLR



#	b	b ⁺⁺	b*	b ^{*++}	b ⁰	b ⁰⁺⁺	Seq.	y	y ⁺⁺	y*	y ^{*++}	y ⁰	y ⁰⁺⁺	#
1	114.0913	57.5493					L							14
2	201.1234	101.0653			183.1128	92.0600	S	1776.8261	888.9167	1759.7996	880.4034	1758.8156	879.9114	13
3	361.1540	181.0806			343.1435	172.0754	C	1689.7941	845.4007	1672.7676	836.8874	1671.7836	836.3954	12
4	432.1911	216.5992			414.1806	207.5939	A	1529.7635	765.3854	1512.7369	756.8721	1511.7529	756.3801	11
5	561.2337	281.1205			543.2232	272.1152	E	1458.7264	729.8668	1441.6998	721.3535	1440.7158	720.8615	10
6	676.2607	338.6340			658.2501	329.6287	D	1329.6838	665.3455	1312.6572	656.8322	1311.6732	656.3402	9
7	1076.4030	538.7051			1058.3924	529.6998	Y	1214.6568	607.8320	1197.6303	599.3188	1196.6463	598.8268	8
8	1189.4870	595.2472			1171.4765	586.2419	L	814.5145	407.7609	797.4880	399.2476	796.5039	398.7556	7
9	1276.5191	638.7632			1258.5085	629.7579	S	701.4304	351.2189	684.4039	342.7056	683.4199	342.2136	6
10	1389.6031	695.3052			1371.5926	686.2999	L	614.3984	307.7028	597.3719	299.1896			5
11	1488.6715	744.8394			1470.6610	735.8341	V	501.3144	251.1608	484.2878	242.6475			4
12	1601.7556	801.3814			1583.7450	792.3762	L	402.2459	201.6266	385.2194	193.1133			3
13	1715.7985	858.4029	1698.7720	849.8896	1697.7880	849.3976	N	289.1619	145.0846	272.1353	136.5713			2
14							R	175.1190	88.0631	158.0924	79.5498			1

Phe 550

TVLGNFAAFVQK



#	b	b ⁺⁺	b*	b ^{*++}	b ⁰	b ⁰⁺⁺	Seq.	y	y ⁺⁺	y*	y ^{*++}	#
1	102.0550	51.5311			84.0444	42.5258	T					12
2	201.1234	101.0653			183.1128	92.0600	V	1430.7467	715.8770	1413.7202	707.3637	11
3	314.2074	157.6074			296.1969	148.6021	L	1331.6783	666.3428	1314.6517	657.8295	10
4	371.2289	186.1181			353.2183	177.1128	G	1218.5942	609.8007	1201.5677	601.2875	9
5	485.2718	243.1395	468.2453	234.6263	467.2613	234.1343	N	1161.5728	581.2900	1144.5462	572.7767	8
6	869.4192	435.2132	852.3927	426.7000	851.4087	426.2080	F	1047.5298	524.2686	1030.5033	515.7553	7
7	940.4563	470.7318	923.4298	462.2185	922.4458	461.7265	A	663.3824	332.1949	646.3559	323.6816	6
8	1011.4934	506.2504	994.4669	497.7371	993.4829	497.2451	A	592.3453	296.6763	575.3188	288.1630	5
9	1158.5619	579.7846	1141.5353	571.2713	1140.5513	570.7793	F	521.3082	261.1577	504.2817	252.6445	4
10	1257.6303	629.3188	1240.6037	620.8055	1239.6197	620.3135	V	374.2398	187.6235	357.2132	179.1103	3
11	1385.6889	693.3481	1368.6623	684.8348	1367.6783	684.3428	Q	275.1714	138.0893	258.1448	129.5761	2
12							K	147.1128	74.0600	130.0863	65.5468	1

Amino acid sequence of RbSA with the altered amino acid residues indicated in red, together with the ESI-MS/MS spectra and fragmentation pathway of each modified peptide

CPF@RbSA

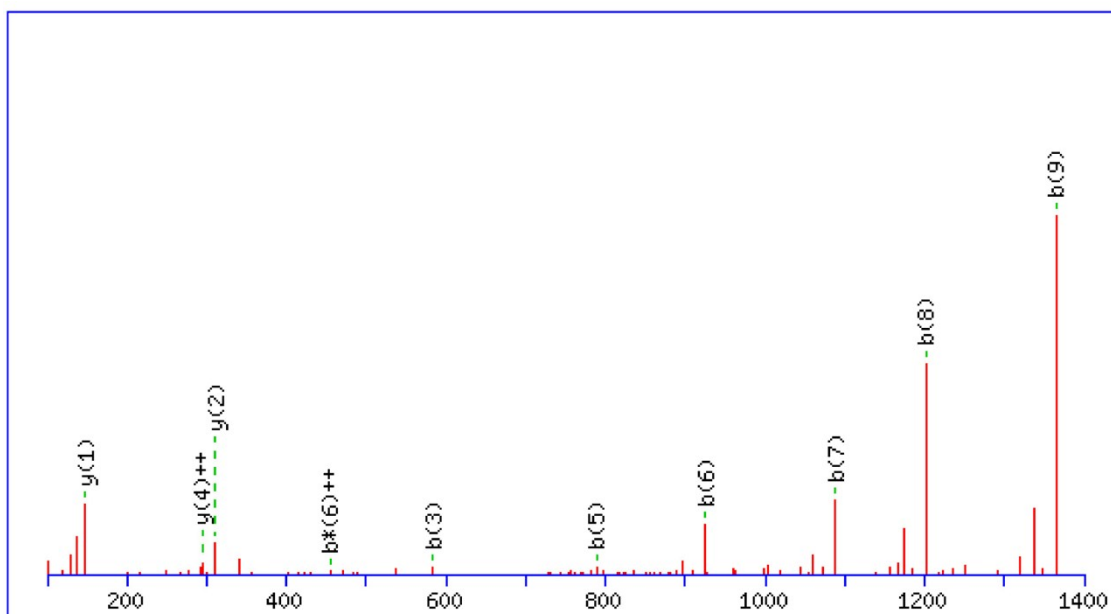
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1  MKWVTFISLL  FLFSSAYSRG  VFRREAHKSE  IAHRFNDVGE  EHFIGLVLIT
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101 LPSLRDITYGD  VADCCCKEKP  ERNECFLHHK  DDKPDLPPFA  RPEADVLCCK
151 FHDDEKATFG  HLYEVARRH  PYSYAPELLY  YAQKYKAILT  ECCEAADKGA
201 CLTPKLDALD  GKSLISAAQE  RLRCASIQKF  GDRAYKAWAL  VRLSQRFPKA
251 DFTDISKIYT  DLTKVHKECC  HGDILLECADD  RADLAKYMCE  HQETISSHLK
301 ECCDKPILEK  AHCIYGLHND  ETPAGLPAVA  EEFVEDKDVC  KNYEEAKDLF
351 LGKFLYEYSR  RHPDYSVLL  LRLGKAYEAT  LKKCCATDDP  HACYAKVLDE
401 FQPLVDEPKN  LVKQNCELYE  QLGDFNFQNA  LLVRYTKKVP  QVSTPTLVEI
451 SRSLGKVGSK  CCKHPEAERL  PCVEDLSVV  LNRLCVLHEK  TPVSEKVTKC
501 CSESLVDRRP  CFSALGPDET  YVPKEFNAET  FTFHADICTL  PETERKIKKQ
551 TALVELVKHK  PHATNDQLKT  VVGFEFTALLD  KCCSAEDKEA  CFAVEGPKLV
601 ESSKATLG

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Phe 134

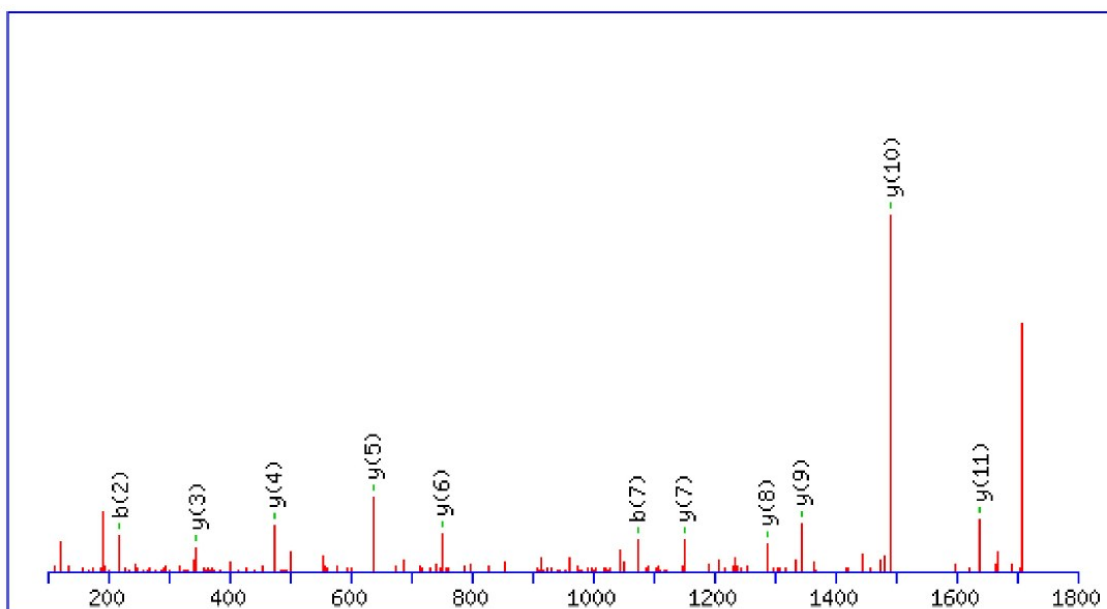
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#	b	b ⁺⁺	b [*]	b ^{*++}	Seq.	y	y ⁺⁺	y ⁰	y ⁰⁺⁺	#
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2	200.1394	100.5733	183.1128	92.0600	A	1383.6045	692.3059	1365.5939	683.3006	9
3	584.2867	292.6470	567.2602	284.1337	F	1312.5673	656.7873	1294.5568	647.7820	8
4	731.3552	366.1812	714.3286	357.6679	F	928.4199	464.7136	910.4094	455.7083	7
5	788.3766	394.6920	771.3501	386.1787	G	781.3515	391.1794	763.3410	382.1741	6
6	925.4355	463.2214	908.4090	454.7081	H	724.3301	362.6687	706.3195	353.6634	5
7	1088.4989	544.7531	1071.4723	536.2398	Y	587.2712	294.1392	569.2606	285.1339	4
8	1201.5829	601.2951	1184.5564	592.7818	L	424.2078	212.6076	406.1973	203.6023	3
9	1364.6463	682.8268	1347.6197	674.3135	Y	311.1238	156.0655	293.1132	147.0602	2

Tyr 138

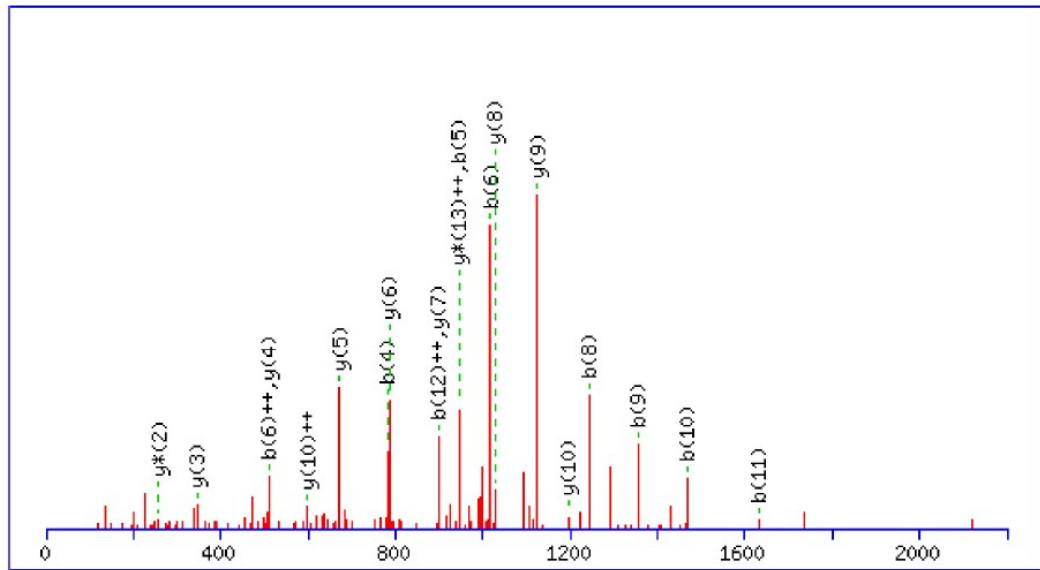
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#	b	b ⁺⁺	b ⁰	b ⁰⁺⁺	Seq.	y	y ⁺⁺	y [*]	y ^{*++}	y ⁰	y ⁰⁺⁺	#
1	72.0444	36.5258			A							12
2	219.1128	110.0600			F	1638.7740	819.8906	1621.7474	811.3774	1620.7634	810.8853	11
3	366.1812	183.5942			F	1491.7056	746.3564	1474.6790	737.8431	1473.6950	737.3511	10
4	423.2027	212.1050			G	1344.6372	672.8222	1327.6106	664.3089	1326.6266	663.8169	9
5	560.2616	280.6344			H	1287.6157	644.3115	1270.5891	635.7982	1269.6051	635.3062	8
6	960.4039	480.7056			Y	1150.5568	575.7820	1133.5302	567.2688	1132.5462	566.7767	7
7	1073.4880	537.2476			L	750.4145	375.7109	733.3879	367.1976	732.4039	366.7056	6
8	1236.5513	618.7793			Y	637.3304	319.1688	620.3039	310.6556	619.3198	310.1636	5
9	1365.5939	683.3006	1347.5833	674.2953	E	474.2671	237.6372	457.2405	229.1239	456.2565	228.6319	4
10	1464.6623	732.8348	1446.6517	723.8295	V	345.2245	173.1159	328.1979	164.6026			3
11	1535.6994	768.3533	1517.6889	759.3481	A	246.1561	123.5817	229.1295	115.0684			2
12					R	175.1190	88.0631	158.0924	79.5498			1

Phe 149

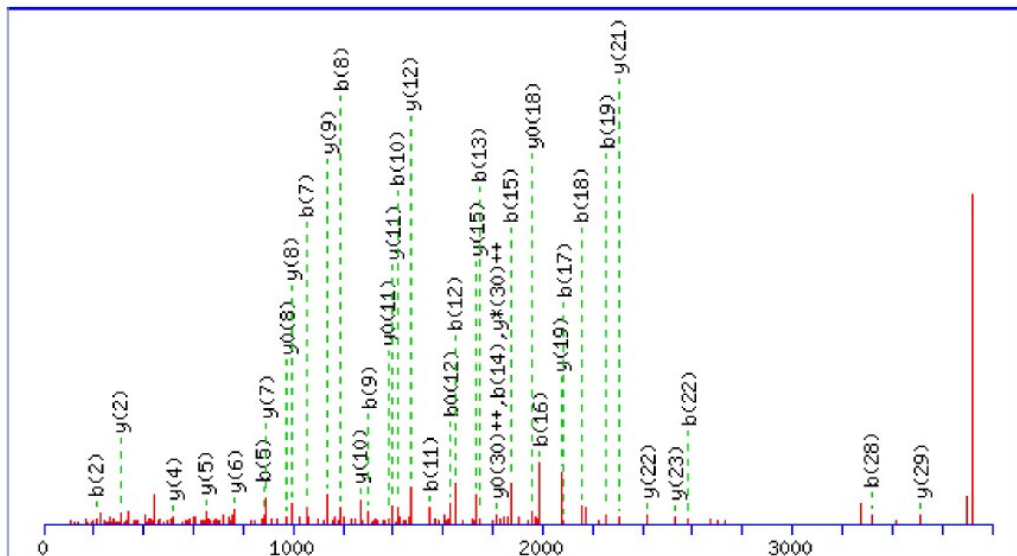
HPYFYAPELLYYAQK



#	b	b ⁺⁺	b [*]	b ^{*++}	b ⁰	b ⁰⁺⁺	Seq.	y	y ⁺⁺	y [*]	y ^{*++}	y ⁰	y ⁰⁺⁺	#
1	138.0662	69.5367					H							15
2	235.1190	118.0631					P	2002.9626	1001.9849	1985.9360	993.4716	1984.9520	992.9796	14
3	398.1823	199.5948					Y	1905.9098	953.4585	1888.8833	944.9453	1887.8992	944.4533	13
4	782.3297	391.6685					F	1742.8465	871.9269	1725.8199	863.4136	1724.8359	862.9216	12
5	945.3930	473.2001					Y	1358.6991	679.8532	1341.6725	671.3399	1340.6885	670.8479	11
6	1016.4301	508.7187					A	1195.6358	598.3215	1178.6092	589.8082	1177.6252	589.3162	10
7	1113.4829	557.2451					P	1124.5986	562.8030	1107.5721	554.2897	1106.5881	553.7977	9
8	1242.5255	621.7664			1224.5149	612.7611	E	1027.5459	514.2766	1010.5193	505.7633	1009.5353	505.2713	8
9	1355.6095	678.3084			1337.5990	669.3031	L	898.5033	449.7553	881.4767	441.2420			7
10	1468.6936	734.8504			1450.6830	725.8452	L	785.4192	393.2132	768.3927	384.7000			6
11	1631.7569	816.3821			1613.7464	807.3768	Y	672.3352	336.6712	655.3086	328.1579			5
12	1794.8203	897.9138			1776.8097	888.9085	Y	509.2718	255.1396	492.2453	246.6263			4
13	1865.8574	933.4323			1847.8468	924.4270	A	346.2085	173.6079	329.1819	165.0946			3
14	1993.9160	997.4616	1976.8894	988.9483	1975.9054	988.4563	Q	275.1714	138.0893	258.1448	129.5761			2
15							K	147.1128	74.0600	130.0863	65.5468			1

Tyr 291

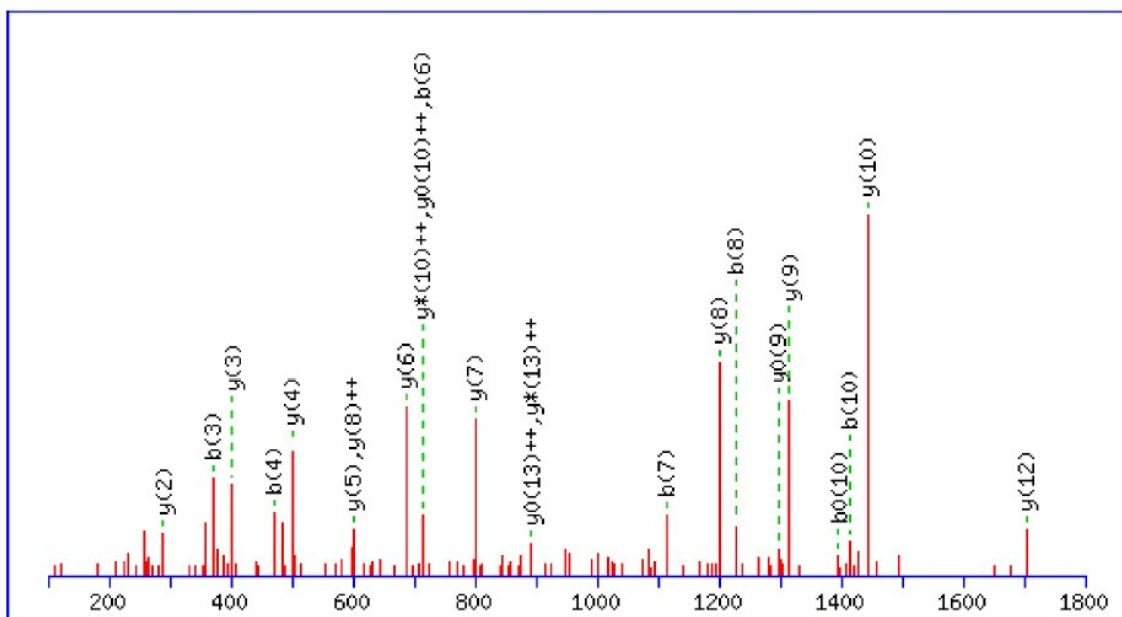
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#	b	b ⁺⁺	b [*]	b ^{*++}	b ⁰	b ⁰⁺⁺	Seq.	y	y ⁺⁺	y [*]	y ^{*++}	y ⁰	y ⁰⁺⁺	#
1	72.0444	36.5258					A							31
2	209.1033	105.0553					H	3650.6566	1825.8320	3633.6301	1817.3187	3632.6461	1816.8267	30
3	369.1340	185.0706					C	3513.5977	1757.3025	3496.5712	1748.7892	3495.5872	1748.2972	29
4	482.2180	241.6126					I	3353.5671	1677.2872	3336.5405	1668.7739	3335.5565	1668.2819	28
5	882.3603	441.6838					Y	3240.4830	1620.7452	3223.4565	1612.2319	3222.4725	1611.7399	27
6	939.3818	470.1945					G	2840.3407	1420.6740	2823.3142	1412.1607	2822.3302	1411.6687	26
7	1052.4659	526.7366					L	2783.3193	1392.1633	2766.2927	1383.6500	2765.3087	1383.1580	25
8	1189.5248	595.2660					H	2670.2352	1335.6212	2653.2086	1327.1080	2652.2246	1326.6159	24
9	1303.5677	652.2875	1286.5411	643.7742			N	2533.1763	1267.0918	2516.1497	1258.5785	2515.1657	1258.0865	23
10	1418.5946	709.8010	1401.5681	701.2877	1400.5841	700.7957	D	2419.1333	1210.0703	2402.1068	1201.5570	2401.1228	1201.0650	22
11	1547.6372	774.3223	1530.6107	765.8090	1529.6267	765.3170	E	2304.1064	1152.5568	2287.0799	1144.0436	2286.0958	1143.5516	21
12	1648.6849	824.8461	1631.6584	816.3328	1630.6743	815.8408	T	2175.0638	1088.0355	2158.0373	1079.5223	2157.0532	1079.0303	20
13	1745.7377	873.3725	1728.7111	864.8592	1727.7271	864.3672	P	2074.0161	1037.5117	2056.9896	1028.9984	2056.0056	1028.5064	19
14	1816.7748	908.8910	1799.7482	900.3778	1798.7642	899.8857	A	1976.9634	988.9853	1959.9368	980.4720	1958.9528	979.9800	18
15	1873.7962	937.4018	1856.7697	928.8885	1855.7857	928.3965	G	1905.9263	953.4668	1888.8997	944.9535	1887.9157	944.4615	17
16	1986.8803	993.9438	1969.8538	985.4305	1968.8697	984.9385	L	1848.9048	924.9560	1831.8782	916.4428	1830.8942	915.9508	16
17	2083.9331	1042.4702	2066.9065	1033.9569	2065.9225	1033.4649	P	1735.8207	868.4140	1718.7942	859.9007	1717.8102	859.4087	15
18	2154.9702	1077.9887	2137.9436	1069.4755	2136.9596	1068.9834	A	1638.7680	819.8876	1621.7414	811.3743	1620.7574	810.8823	14
19	2254.0386	1127.5229	2237.0121	1119.0097	2236.0280	1118.5177	V	1567.7309	784.3691	1550.7043	775.8558	1549.7203	775.3638	13
20	2325.0757	1163.0415	2308.0492	1154.5282	2307.0652	1154.0362	A	1468.6624	734.8349	1451.6359	726.3216	1450.6519	725.8296	12
21	2454.1183	1227.5628	2437.0918	1219.0495	2436.1077	1218.5575	E	1397.6253	699.3163	1380.5988	690.8030	1379.6148	690.3110	11
22	2583.1609	1292.0841	2566.1344	1283.5708	2565.1503	1283.0788	E	1268.5827	634.7950	1251.5562	626.2817	1250.5722	625.7897	10
23	2730.2293	1365.6183	2713.2028	1357.1050	2712.2188	1356.6130	F	1139.5401	570.2737	1122.5136	561.7604	1121.5296	561.2684	9
24	2829.2977	1415.1525	2812.2712	1406.6392	2811.2872	1406.1472	V	992.4717	496.7395	975.4452	488.2262	974.4612	487.7342	8
25	2958.3403	1479.6738	2941.3138	1471.1605	2940.3298	1470.6685	E	893.4033	447.2053	876.3768	438.6920	875.3927	438.2000	7

Tyr 452

LPCVEDLSVVLNR



#	b	b ⁺⁺	b*	b ^{*++}	b ⁰	b ⁰⁺⁺	Seq.	y	y ⁺⁺	y*	y ^{*++}	y ⁰	y ⁰⁺⁺	#
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2	211.1441	106.0757					P	1800.8625	900.9349	1783.8360	892.4216	1782.8520	891.9296	13
3	371.1748	186.0910					C	1703.8098	852.4085	1686.7832	843.8952	1685.7992	843.4032	12
4	470.2432	235.6252					V	1543.7791	772.3932	1526.7526	763.8799	1525.7686	763.3879	11
5	599.2858	300.1465			581.2752	291.1412	E	1444.7107	722.8590	1427.6842	714.3457	1426.7001	713.8537	10
6	714.3127	357.6600			696.3021	348.6547	D	1315.6681	658.3377	1298.6416	649.8244	1297.6575	649.3324	9
7	1114.4550	557.7311			1096.4444	548.7259	Y	1200.6412	600.8242	1183.6146	592.3109	1182.6306	591.8189	8
8	1227.5391	614.2732			1209.5285	605.2679	L	800.4989	400.7531	783.4723	392.2398	782.4883	391.7478	7
9	1314.5711	657.7892			1296.5605	648.7839	S	687.4148	344.2110	670.3883	335.6978	669.4042	335.2058	6
10	1413.6395	707.3234			1395.6290	698.3181	V	600.3828	300.6950	583.3562	292.1817			5
11	1512.7079	756.8576			1494.6974	747.8523	V	501.3144	251.1608	484.2878	242.6475			4
12	1625.7920	813.3996			1607.7814	804.3944	L	402.2459	201.6266	385.2194	193.1133			3
13	1739.8349	870.4211	1722.8084	861.9078	1721.8244	861.4158	N	289.1619	145.0846	272.1353	136.5713			2
14							R	175.1190	88.0631	158.0924	79.5498			1

Amino acid sequence of RtSA with the altered amino acid residues indicated in red, together with the ESI-MS/MS spectra and fragmentation pathway of each modified peptide

CPF/RtSA

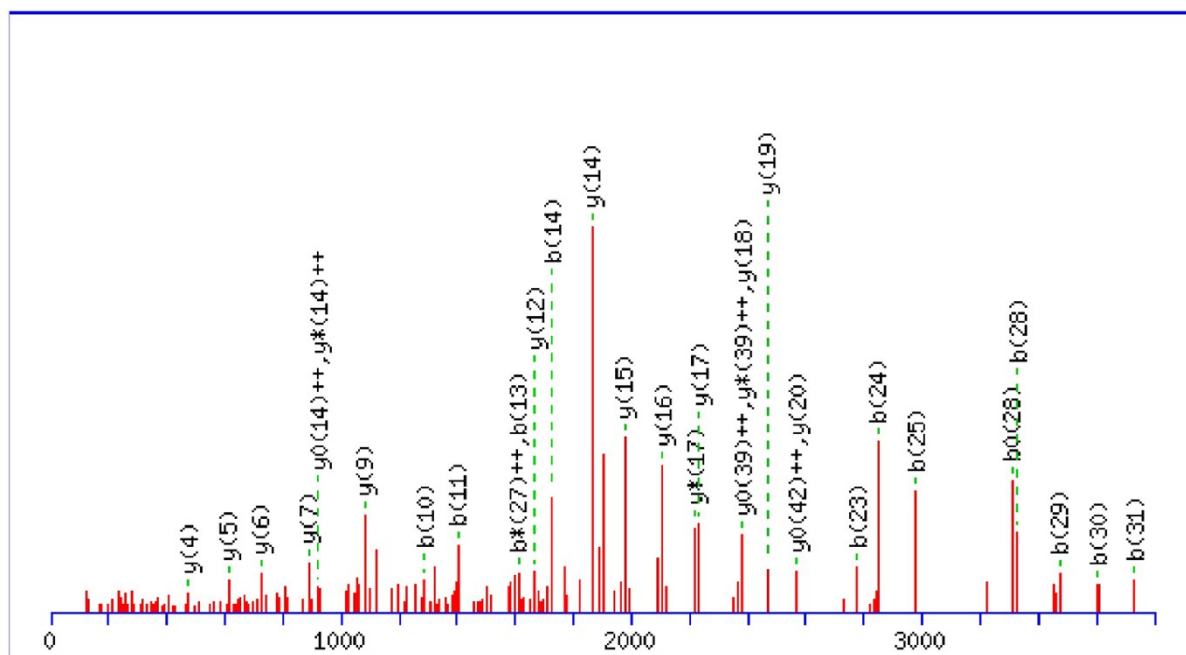
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1  MKWVTFLLLL FISGSAFSRG VFRREAHKSE IAHRFKDLGE QHFKGLVLIA
51  FSQYLQKCPY EEHIKLVQEV TDFAKTCVAD ENAENCDSKI HTLFGDKLCA
101 IPKLRDNYGE LADCCAKQEP ERNECFLQHK DDNPNLPPFQ RPEAEAMCTS
151 FQENPTSFLG HYLHEVARRH PYTYAPELLY YAEKTNEVLT QCCTESDKAA
201 CLTPKLDAVK EKALVAAVRQ RMKCSSMQRF GERAFKAWAV ARMSQRFPNA
251 EFAEITKLAT DVTKINKECC HGDILLECADD RAELAKYMCE NQATISSKLQ
301 ACCDKPVLQK SQCLAEIEHD NIPADLPSIA ADFVEDKEVC KNYAEAKDVF
351 LGTFLYEYSR RHPDYSVSLL LRLAKKYEAT LEKCCAEGDP PACYGTVLAE
401 FQPLVEEPKN LVKTNCELYE KLGEYGFQNA VLVRYTQKAP QVSTPTLVEA
451 ARNLGRVGTK CCTLPEAQRL PCVEDTLSAI LNRLCVLHEK TPVSEKVTKC
501 CSGSLVERRP CFSALTVDET YVPKEFKAET FTTHSDICTL PDKEKQIKKQ
551 TALAEIVKHK PKATEDQLKT VMGDFAQFVD KCCKAADKDN CFATEGPNLV
601 ARSKEALA

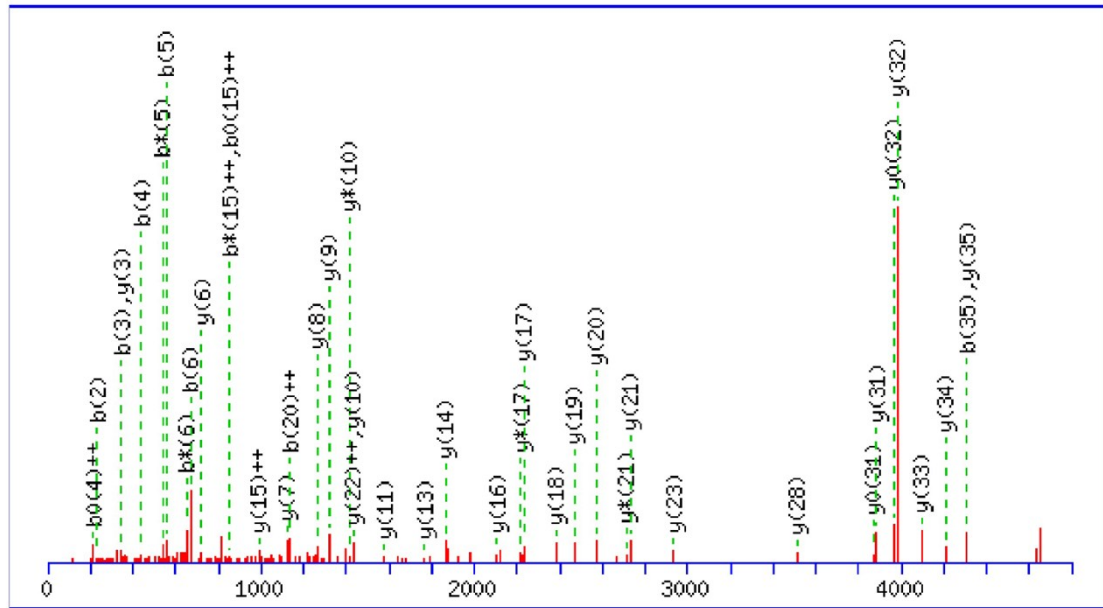
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Phe 134

NECFLQH~~K~~DDNP~~N~~LPPFQRPEAEAMCTSFQENPTS~~F~~LG~~H~~YLHEVAR



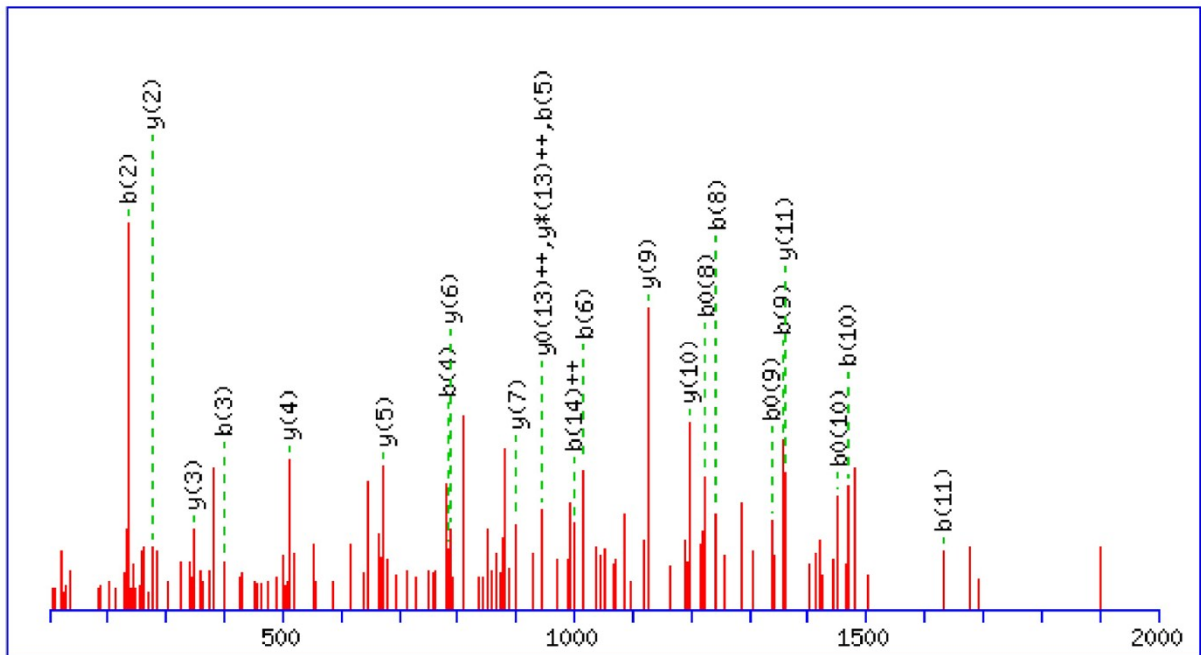
#	b	b ⁺⁺	b*	b ^{*++}	b ⁰	b ⁰⁺⁺	Seq.	y	y ⁺⁺	y*	y ^{*++}	y ⁰	y ⁰⁺⁺	#
1	115.0502	58.0287	98.0237	49.5155			N							46
2	244.0928	122.5500	227.0662	114.0368	226.0822	113.5448	E	5594.5416	2797.7744	5577.5150	2789.2612	5576.5310	2788.7691	45
3	404.1234	202.5654	387.0969	194.0521	386.1129	193.5601	C	5465.4990	2733.2531	5448.4724	2724.7399	5447.4884	2724.2479	44
4	551.1919	276.0996	534.1653	267.5863	533.1813	267.0943	F	5305.4683	2653.2378	5288.4418	2644.7245	5287.4578	2644.2325	43
5	664.2759	332.6416	647.2494	324.1283	646.2654	323.6363	L	5158.3999	2579.7036	5141.3734	2571.1903	5140.3894	2570.6983	42
6	792.3345	396.6709	775.3080	388.1576	774.3239	387.6656	Q	5045.3159	2523.1616	5028.2893	2514.6483	5027.3053	2514.1563	41
7	929.3934	465.2003	912.3669	456.6871	911.3828	456.1951	H	4917.2573	2459.1323	4900.2307	2450.6190	4899.2467	2450.1270	40
8	1057.4884	529.2478	1040.4618	520.7346	1039.4778	520.2425	K	4780.1984	2390.6028	4763.1718	2382.0896	4762.1878	2381.5975	39
9	1172.5153	586.7613	1155.4888	578.2480	1154.5048	577.7560	D	4652.1034	2326.5553	4635.0769	2318.0421	4634.0928	2317.5501	38
10	1287.5423	644.2748	1270.5157	635.7615	1269.5317	635.2695	D	4537.0765	2269.0419	4520.0499	2260.5286	4519.0659	2260.0366	37
11	1401.5852	701.2962	1384.5586	692.7830	1383.5746	692.2910	N	4422.0495	2211.5284	4405.0230	2203.0151	4404.0390	2202.5231	36
12	1498.6380	749.8226	1481.6114	741.3093	1480.6274	740.8173	P	4308.0066	2154.5069	4290.9801	2145.9937	4289.9960	2145.5017	35
13	1612.6809	806.8441	1595.6543	798.3308	1594.6703	797.8388	N	4210.9538	2105.9806	4193.9273	2097.4673	4192.9433	2096.9753	34
14	1725.7649	863.3861	1708.7384	854.8728	1707.7544	854.3808	L	4096.9109	2048.9591	4079.8844	2040.4458	4078.9003	2039.9538	33
15	1822.8177	911.9125	1805.7912	903.3992	1804.8071	902.9072	P	3983.8268	1992.4171	3966.8003	1983.9038	3965.8163	1983.4118	32
16	1919.8705	960.4389	1902.8439	951.9256	1901.8599	951.4336	P	3886.7741	1943.8907	3869.7475	1935.3774	3868.7635	1934.8854	31
17	2066.9389	1033.9731	2049.9123	1025.4598	2048.9283	1024.9678	F	3789.7213	1895.3643	3772.6948	1886.8510	3771.7108	1886.3590	30
18	2194.9975	1098.0024	2177.9709	1089.4891	2176.9869	1088.9971	Q	3642.6529	1821.8301	3625.6264	1813.3168	3624.6423	1812.8248	29
19	2351.0986	1176.0529	2334.0720	1167.5397	2333.0880	1167.0476	P	3514.5943	1757.8008	3497.5678	1749.2875	3496.5838	1748.7955	28
20	2448.1513	1224.5793	2431.1248	1216.0660	2430.1408	1215.5740	R	3358.4932	1679.7502	3341.4667	1671.2370	3340.4826	1670.7450	27
21	2577.1939	1289.1006	2560.1674	1280.5873	2559.1834	1280.0953	E	3261.4404	1631.2239	3244.4139	1622.7106	3243.4299	1622.2186	26
22	2648.2310	1324.6192	2631.2045	1316.1059	2630.2205	1315.6139	A	3132.3979	1566.7026	3115.3713	1558.1893	3114.3873	1557.6973	25
23	2777.2736	1389.1405	2760.2471	1380.6272	2759.2631	1380.1352	E	3061.3607	1531.1840	3044.3342	1522.6707	3043.3502	1522.1787	24
24	2848.3108	1424.6590	2831.2842	1416.1457	2830.3002	1415.6537	A	2932.3181	1466.6627	2915.2916	1458.1494	2914.3076	1457.6574	23
25	2979.3512	1490.1793	2962.3247	1481.6660	2961.3407	1481.1740	M	2861.2810	1431.1442	2844.2545	1422.6309	2843.2705	1422.1389	22
26	3139.3819	1570.1946	3122.3553	1561.6813	3121.3713	1561.1893	C	2730.2405	1365.6239	2713.2140	1357.1106	2712.2300	1356.6186	21
27	3240.4296	1620.7184	3223.4030	1612.2051	3222.4190	1611.7131	T	2570.2099	1285.6086	2553.1834	1277.0953	2552.1993	1276.6033	20
28	3327.4616	1664.2344	3310.4350	1655.7212	3309.4510	1655.2292	S	2469.1622	1235.0847	2452.1357	1226.5715	2451.1517	1226.0795	19
29	3474.5300	1737.7686	3457.5035	1729.2554	3456.5194	1728.7634	F	2382.1302	1191.5687	2365.1036	1183.0555	2364.1196	1182.5635	18
30	3602.5886	1801.7979	3585.5620	1793.2847	3584.5780	1792.7926	Q	2235.0618	1118.0345	2218.0352	1109.5213	2217.0512	1109.0292	17
31	3731.6312	1866.3192	3714.6046	1857.8060	3713.6206	1857.3139	E	2107.0032	1054.0052	2089.9767	1045.4920	2088.9926	1045.0000	16
32	3845.6741	1923.3407	3828.6476	1914.8274	3827.6635	1914.3354	N	1977.9606	989.4839	1960.9341	980.9707	1959.9500	980.4787	15
33	3942.7269	1971.8671	3925.7003	1963.3538	3924.7163	1962.8618	P	1863.9177	932.4625	1846.8911	923.9492	1845.9071	923.4572	14
34	4043.7745	2022.3909	4026.7480	2013.8776	4025.7640	2013.3856	T	1766.8649	883.9361	1749.8384	875.4228	1748.8544	874.9308	13
35	4130.8066	2065.9069	4113.7800	2057.3937	4112.7960	2056.9016	S	1665.8172	833.4123	1648.7907	824.8990	1647.8067	824.4070	12
36	4514.9540	2257.9806	4497.9274	2249.4673	4496.9434	2248.9753	F	1578.7852	789.8962	1561.7587	781.3830	1560.7746	780.8910	11
37	4628.0380	2314.5227	4611.0115	2306.0094	4610.0275	2305.5174	L	1194.6378	597.8225	1177.6113	589.3093	1176.6273	588.8173	10
38	4685.0595	2343.0334	4668.0329	2334.5201	4667.0489	2334.0281	G	1081.5538	541.2805	1064.5272	532.7672	1063.5432	532.2752	9
39	4822.1184	2411.5628	4805.0919	2403.0496	4804.1078	2402.5576	H	1024.5323	512.7698	1007.5057	504.2565	1006.5217	503.7645	8
40	4985.1817	2493.0945	4968.1552	2484.5812	4967.1712	2484.0892	Y	887.4734	444.2403	870.4468	435.7271	869.4628	435.2350	7
41	5098.2658	2549.6365	5081.2393	2541.1233	5080.2552	2540.6313	L	724.4100	362.7087	707.3835	354.1954	706.3995	353.7034	6
42	5235.3247	2618.1660	5218.2982	2609.6527	5217.3142	2609.1607	H	611.3260	306.1666	594.2994	297.6534	593.3154	297.1613	5
43	5364.3673	2682.6873	5347.3408	2674.1740	5346.3567	2673.6820	E	474.2671	237.6372	457.2405	229.1239	456.2565	228.6319	4
44	5463.4357	2732.2215	5446.4092	2723.7082	5445.4252	2723.2162	V	345.2245	173.1159	328.1979	164.6026			3
45	5534.4728	2767.7401	5517.4463	2759.2268	5516.4623	2758.7348	A	246.1561	123.5817	229.1295	115.0684			2
46							R	175.1190	88.0631	158.0924	79.5498			1



26	2987.2934	1494.1504	2970.2669	1485.6371	2969.2829	1485.1451	T	1766.8649	883.9361	1749.8384	875.4228	1748.8544	874.9308	13
27	3074.3255	1537.6664	3057.2989	1529.1531	3056.3149	1528.6611	S	1665.8172	833.4123	1648.7907	824.8990	1647.8067	824.4070	12
28	3221.3939	1611.2006	3204.3673	1602.6873	3203.3833	1602.1953	F	1578.7852	789.8962	1561.7587	781.3830	1560.7746	780.8910	11
29	3334.4780	1667.7426	3317.4514	1659.2293	3316.4674	1658.7373	L	1431.7168	716.3620	1414.6902	707.8488	1413.7062	707.3568	10
30	3391.4994	1696.2533	3374.4729	1687.7401	3373.4889	1687.2481	G	1318.6327	659.8200	1301.6062	651.3067	1300.6222	650.8147	9
31	3528.5583	1764.7828	3511.5318	1756.2695	3510.5478	1755.7775	H	1261.6113	631.3093	1244.5847	622.7960	1243.6007	622.3040	8
32	3928.7006	1964.8540	3911.6741	1956.3407	3910.6901	1955.8487	Y	1124.5524	562.7798	1107.5258	554.2665	1106.5418	553.7745	7
33	4041.7847	2021.3960	4024.7582	2012.8827	4023.7741	2012.3907	L	724.4100	362.7087	707.3835	354.1954	706.3995	353.7034	6
34	4178.8436	2089.9254	4161.8171	2081.4122	4160.8331	2080.9202	H	611.3260	306.1666	594.2994	297.6534	593.3154	297.1613	5
35	4307.8862	2154.4467	4290.8597	2145.9335	4289.8756	2145.4415	E	474.2671	237.6372	457.2405	229.1239	456.2565	228.6319	4
36	4406.9546	2203.9809	4389.9281	2195.4677	4388.9441	2194.9757	V	345.2245	173.1159	328.1979	164.6026			3
37	4477.9917	2239.4995	4460.9652	2230.9862	4459.9812	2230.4942	A	246.1561	123.5817	229.1295	115.0684			2
38							R	175.1190	88.0631	158.0924	79.5498			1

Phe 149

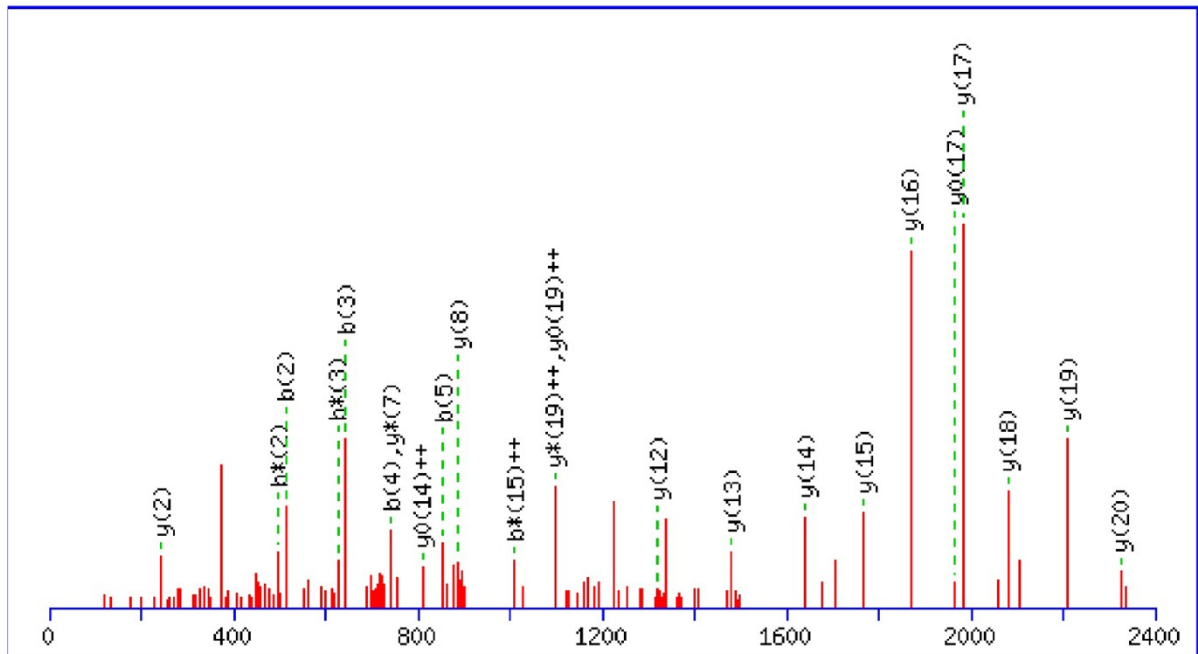
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4	782.3297	391.6685			F	1743.8305	872.4189	1726.8039	863.9056	1725.8199	863.4136	12
5	945.3930	473.2001			Y	1359.6831	680.3452	1342.6565	671.8319	1341.6725	671.3399	11
6	1016.4301	508.7187			A	1196.6198	598.8135	1179.5932	590.3002	1178.6092	589.8082	10
7	1113.4829	557.2451			P	1125.5827	563.2950	1108.5561	554.7817	1107.5721	554.2897	9
8	1242.5255	621.7664	1224.5149	612.7611	E	1028.5299	514.7686	1011.5033	506.2553	1010.5193	505.7633	8
9	1355.6095	678.3084	1337.5990	669.3031	L	899.4873	450.2473	882.4607	441.7340	881.4767	441.2420	7
10	1468.6936	734.8504	1450.6830	725.8452	L	786.4032	393.7053	769.3767	385.1920	768.3927	384.7000	6
11	1631.7569	816.3821	1613.7464	807.3768	Y	673.3192	337.1632	656.2926	328.6499	655.3086	328.1579	5
12	1794.8203	897.9138	1776.8097	888.9085	Y	510.2558	255.6316	493.2293	247.1183	492.2453	246.6263	4
13	1865.8574	933.4323	1847.8468	924.4270	A	347.1925	174.0999	330.1660	165.5866	329.1819	165.0946	3
14	1994.9000	997.9536	1976.8894	988.9483	E	276.1554	138.5813	259.1288	130.0681	258.1448	129.5761	2
15					K	147.1128	74.0600	130.0863	65.5468			1

Tyr 161

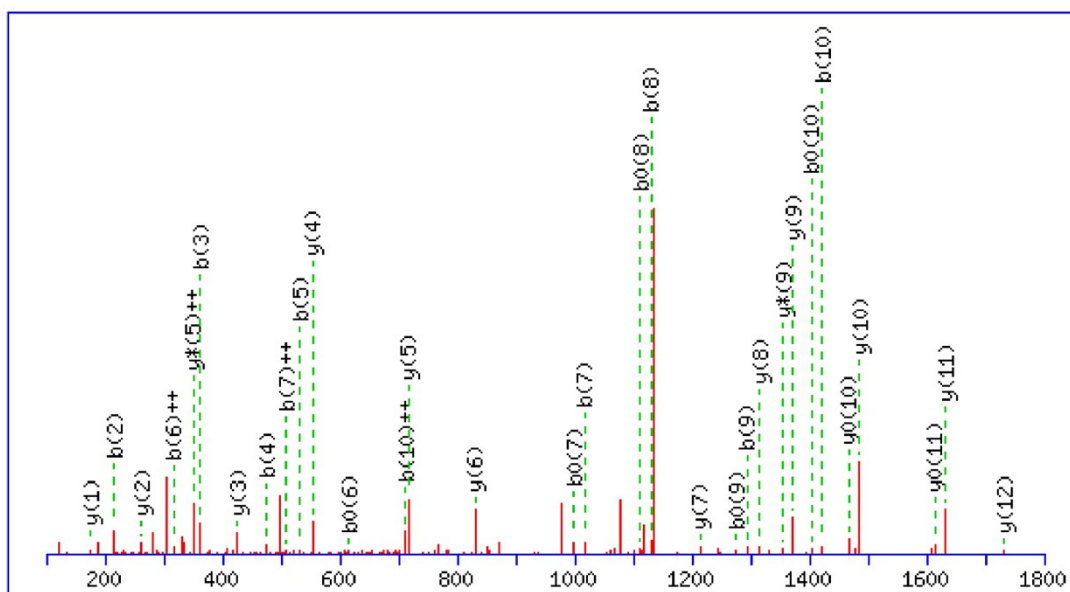
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2	515.1925	258.0999	498.1660	249.5866			N	2325.0519	1163.0296	2308.0254	1154.5163	2307.0414	1154.0243	20
3	644.2351	322.6212	627.2086	314.1079	626.2245	313.6159	E	2211.0090	1106.0081	2193.9825	1097.4949	2192.9985	1097.0029	19
4	743.3035	372.1554	726.2770	363.6421	725.2930	363.1501	V	2081.9664	1041.4869	2064.9399	1032.9736	2063.9559	1032.4816	18
5	856.3876	428.6974	839.3610	420.1842	838.3770	419.6921	L	1982.8980	991.9526	1965.8715	983.4394	1964.8874	982.9474	17
6	957.4353	479.2213	940.4087	470.7080	939.4247	470.2160	T	1869.8139	935.4106	1852.7874	926.8973	1851.8034	926.4053	16
7	1085.4938	543.2506	1068.4673	534.7373	1067.4833	534.2453	Q	1768.7663	884.8868	1751.7397	876.3735	1750.7557	875.8815	15
8	1245.5245	623.2659	1228.4979	614.7526	1227.5139	614.2606	C	1640.7077	820.8575	1623.6811	812.3442	1622.6971	811.8522	14
9	1405.5551	703.2812	1388.5286	694.7679	1387.5446	694.2759	C	1480.6770	740.8422	1463.6505	732.3289	1462.6665	731.8369	13
10	1506.6028	753.8050	1489.5763	745.2918	1488.5923	744.7998	T	1320.6464	660.8268	1303.6198	652.3136	1302.6358	651.8216	12
11	1635.6454	818.3263	1618.6189	809.8131	1617.6348	809.3211	E	1219.5987	610.3030	1202.5722	601.7897	1201.5882	601.2977	11
12	1722.6774	861.8424	1705.6509	853.3291	1704.6669	852.8371	S	1090.5561	545.7817	1073.5296	537.2684	1072.5456	536.7764	10
13	1837.7044	919.3558	1820.6778	910.8426	1819.6938	910.3505	D	1003.5241	502.2657	986.4975	493.7524	985.5135	493.2604	9
14	1965.7993	983.4033	1948.7728	974.8900	1947.7888	974.3980	K	888.4972	444.7522	871.4706	436.2389	870.4866	435.7469	8
15	2036.8365	1018.9219	2019.8099	1010.4086	2018.8259	1009.9166	A	760.4022	380.7047	743.3756	372.1915	742.3916	371.6994	7
16	2107.8736	1054.4404	2090.8470	1045.9271	2089.8630	1045.4351	A	689.3651	345.1862	672.3385	336.6729	671.3545	336.1809	6
17	2267.9042	1134.4557	2250.8777	1125.9425	2249.8937	1125.4505	C	618.3280	309.6676	601.3014	301.1543	600.3174	300.6623	5
18	2380.9883	1190.9978	2363.9617	1182.4845	2362.9777	1181.9925	L	458.2973	229.6523	441.2708	221.1390	440.2867	220.6470	4
19	2482.0360	1241.5216	2465.0094	1233.0083	2464.0254	1232.5163	T	345.2132	173.1103	328.1867	164.5970	327.2027	164.1050	3
20	2579.0887	1290.0480	2562.0622	1281.5347	2561.0782	1281.0427	P	244.1656	122.5864	227.1390	114.0731			2
21							K	147.1128	74.0600	130.0863	65.5468			1

Phe 330

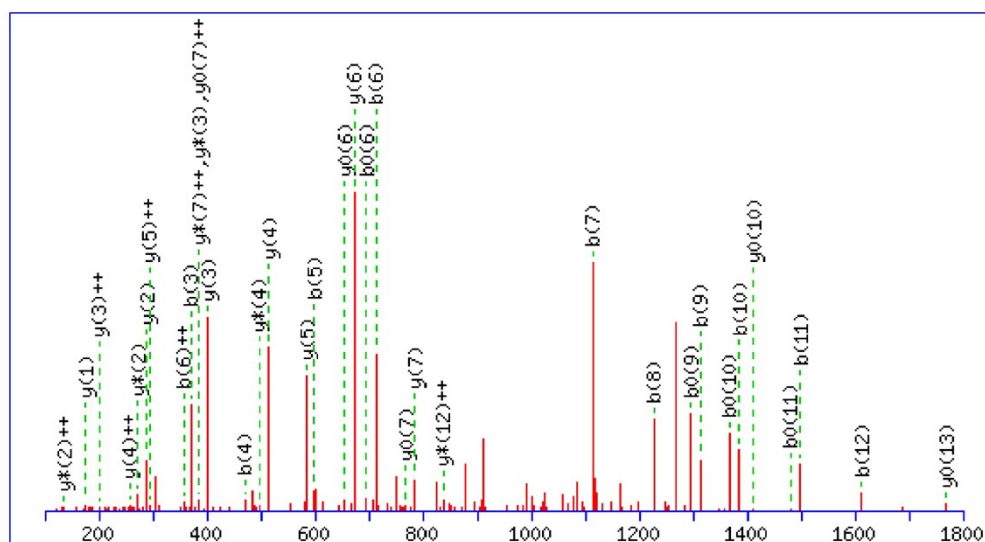
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#	b	b ⁺⁺	b ⁰	b ⁰⁺⁺	Seq.	y	y ⁺⁺	y [*]	y ^{*++}	y ⁰	y ⁰⁺⁺	#
1	116.0342	58.5207	98.0237	49.5155	D							13
2	215.1026	108.0550	197.0921	99.0497	V	1731.8417	866.4245	1714.8152	857.9112	1713.8312	857.4192	12
3	362.1710	181.5892	344.1605	172.5839	F	1632.7733	816.8903	1615.7468	808.3770	1614.7627	807.8850	11
4	475.2551	238.1312	457.2445	229.1259	L	1485.7049	743.3561	1468.6783	734.8428	1467.6943	734.3508	10
5	532.2766	266.6419	514.2660	257.6366	G	1372.6208	686.8141	1355.5943	678.3008	1354.6103	677.8088	9
6	633.3243	317.1658	615.3137	308.1605	T	1315.5994	658.3033	1298.5728	649.7900	1297.5888	649.2980	8
7	1017.4716	509.2395	999.4611	500.2342	F	1214.5517	607.7795	1197.5251	599.2662	1196.5411	598.7742	7
8	1130.5557	565.7815	1112.5451	556.7762	L	830.4043	415.7058	813.3777	407.1925	812.3937	406.7005	6
9	1293.6190	647.3132	1275.6085	638.3079	Y	717.3202	359.1638	700.2937	350.6505	699.3097	350.1585	5
10	1422.6616	711.8345	1404.6511	702.8292	E	554.2569	277.6321	537.2304	269.1188	536.2463	268.6268	4
11	1585.7250	793.3661	1567.7144	784.3608	Y	425.2143	213.1108	408.1878	204.5975	407.2037	204.1055	3
12	1672.7570	836.8821	1654.7464	827.8769	S	262.1510	131.5791	245.1244	123.0659	244.1404	122.5738	2
13					R	175.1190	88.0631	158.0924	79.5498			1

Tyr 452

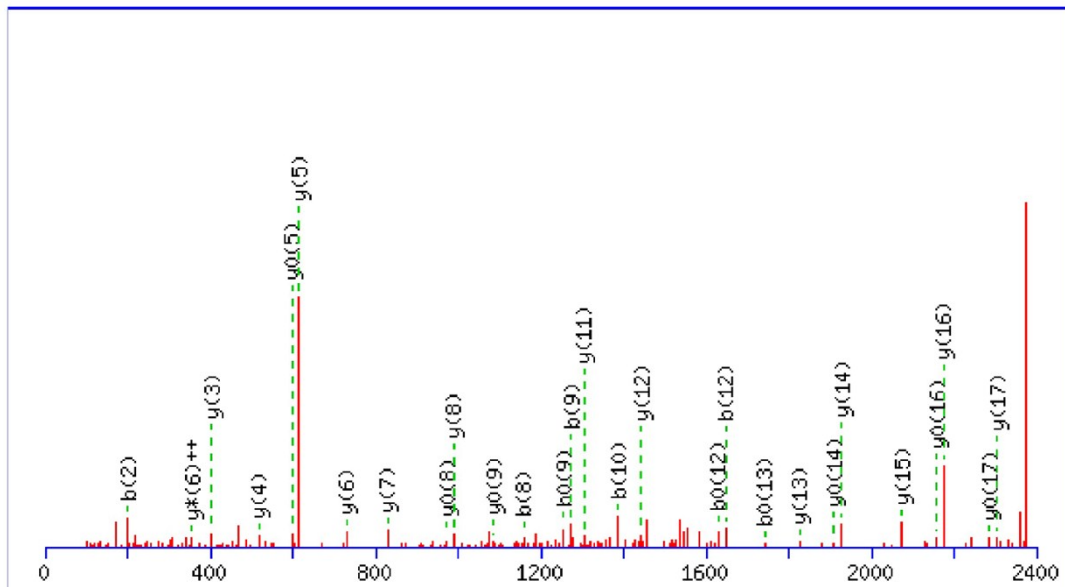
LPCVEDYLSAILNR



#	b	b ⁺⁺	b*	b ^{*++}	b ⁰	b ⁰⁺⁺	Seq.	y	y ⁺⁺	y*	y ^{*++}	y ⁰	y ⁰⁺⁺	#
1	114.0913	57.5493					L							14
2	211.1441	106.0757					P	1786.8469	893.9271	1769.8203	885.4138	1768.8363	884.9218	13
3	371.1748	186.0910					C	1689.7941	845.4007	1672.7676	836.8874	1671.7836	836.3954	12
4	470.2432	235.6252					V	1529.7635	765.3854	1512.7369	756.8721	1511.7529	756.3801	11
5	599.2858	300.1465			581.2752	291.1412	E	1430.6951	715.8512	1413.6685	707.3379	1412.6845	706.8459	10
6	714.3127	357.6600			696.3021	348.6547	D	1301.6525	651.3299	1284.6259	642.8166	1283.6419	642.3246	9
7	1114.4550	557.7311			1096.4444	548.7259	Y	1186.6255	593.8164	1169.5990	585.3031	1168.6150	584.8111	8
8	1227.5391	614.2732			1209.5285	605.2679	L	786.4832	393.7452	769.4567	385.2320	768.4726	384.7400	7
9	1314.5711	657.7892			1296.5605	648.7839	S	673.3991	337.2032	656.3726	328.6899	655.3886	328.1979	6
10	1385.6082	693.3077			1367.5977	684.3025	A	586.3671	293.6872	569.3406	285.1739			5
11	1498.6923	749.8498			1480.6817	740.8445	I	515.3300	258.1686	498.3035	249.6554			4
12	1611.7763	806.3918			1593.7658	797.3865	L	402.2459	201.6266	385.2194	193.1133			3
13	1725.8193	863.4133	1708.7927	854.9000	1707.8087	854.4080	N	289.1619	145.0846	272.1353	136.5713			2
14							R	175.1190	88.0631	158.0924	79.5498			1

Phe 509

AETFT**H**SDICTLPDKEK



#	b	b ⁺⁺	b*	b ^{*++}	b ⁰	b ⁰⁺⁺	Seq.	y	y ⁺⁺	y*	y ^{*++}	y ⁰	y ⁰⁺⁺	#
1	72.0444	36.5258					A							18
2	201.0870	101.0471			183.0764	92.0418	E	2305.0482	1153.0277	2288.0216	1144.5144	2287.0376	1144.0224	17
3	302.1347	151.5710			284.1241	142.5657	T	2176.0056	1088.5064	2158.9790	1079.9931	2157.9950	1079.5011	16
4	449.2031	225.1052			431.1925	216.0999	F	2074.9579	1037.9826	2057.9313	1029.4693	2056.9473	1028.9773	15
5	550.2508	275.6290			532.2402	266.6237	T	1927.8895	964.4484	1910.8629	955.9351	1909.8789	955.4431	14
6	934.3981	467.7027			916.3876	458.6974	F	1826.8418	913.9245	1809.8153	905.4113	1808.8312	904.9193	13
7	1071.4571	536.2322			1053.4465	527.2269	H	1442.6944	721.8508	1425.6679	713.3376	1424.6838	712.8456	12
8	1158.4891	579.7482			1140.4785	570.7429	S	1305.6355	653.3214	1288.6089	644.8081	1287.6249	644.3161	11
9	1273.5160	637.2617			1255.5055	628.2564	D	1218.6035	609.8054	1201.5769	601.2921	1200.5929	600.8001	10
10	1386.6001	693.8037			1368.5895	684.7984	I	1103.5765	552.2919	1086.5500	543.7786	1085.5660	543.2866	9
11	1546.6307	773.8190			1528.6202	764.8137	C	990.4925	495.7499	973.4659	487.2366	972.4819	486.7446	8
12	1647.6784	824.3428			1629.6679	815.3376	T	830.4618	415.7345	813.4353	407.2213	812.4512	406.7293	7
13	1760.7625	880.8849			1742.7519	871.8796	L	729.4141	365.2107	712.3876	356.6974	711.4036	356.2054	6
14	1857.8153	929.4113			1839.8047	920.4060	P	616.3301	308.6687	599.3035	300.1554	598.3195	299.6634	5
15	1972.8422	986.9247			1954.8316	977.9195	D	519.2773	260.1423	502.2508	251.6290	501.2667	251.1370	4
16	2100.9372	1050.9722	2083.9106	1042.4589	2082.9266	1041.9669	K	404.2504	202.6288	387.2238	194.1155	386.2398	193.6235	3
17	2229.9798	1115.4935	2212.9532	1106.9802	2211.9692	1106.4882	E	276.1554	138.5813	259.1288	130.0681	258.1448	129.5761	2
18							K	147.1128	74.0600	130.0863	65.5468			1

Amino acid sequence of SSA with the altered amino acid residues indicated in red, together with the ESI-MS/MS spectra and fragmentation pathway of each modified peptide

CPF/SSA

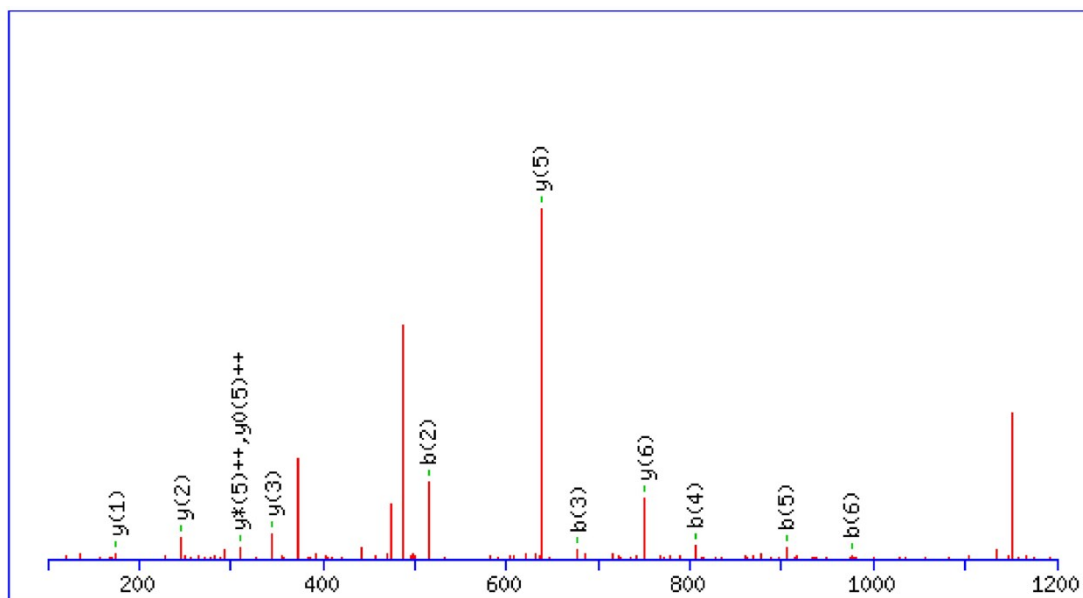
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1  MKWVTFISLL LLFSSAYSRG VFRRDTHKSE IAHRFNDLGE ENFQGLVLIA
51  FSQYLQQCPF DEHVKLKVEL TEFKATCVAD ESHAGCDKSL HTLFGDELCK
101 VATLRETYGD MADCCEKQEP ERNECFLNHK DDSPDLPKLK PEPDTLCAEF
151 KADEKKFWGK YLYEVARRHP YFYAPELLYY ANKYNGVFQE CCQAEDKGAC
201 LLPKIDAMRE KVLASSARQR LRCASIQKFG ERAKAWSVV RLSQKFPKAD
251 FTDVTKIVTD LTKVHKECCH GDLLECADDR ADLAKYICDH QDALSSKLKE
301 CCDKPVLEKS HCIAEVDKDA VPENLPPLTA DFAEDKEVCK NYQEAKDVIL
351 GSYLYEYSRR HPEYAVSVLL RLAKEYEATL EDCCAKEDPH ACYATVFDKL
401 KHLVDEPQNL IKKNCELFK HGEYGFQNAL IVRYTRKAPQ VSTPTLVEIS
451 RSLGKVGTKC CAKPESERMP CTEDLSLIL NRLCVLHEKT PVSEKVTGCC
501 TESLVNRRPC FSDLTLDETY VPKPFDEKFF TFHADICTLP DTEKQIKKQT
551 ALVELLKHKP KATDEQLKTV MENFVAFVDK CCAADDKEGC FVLEGPKLVA
601 STQAALA

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Tyr 137

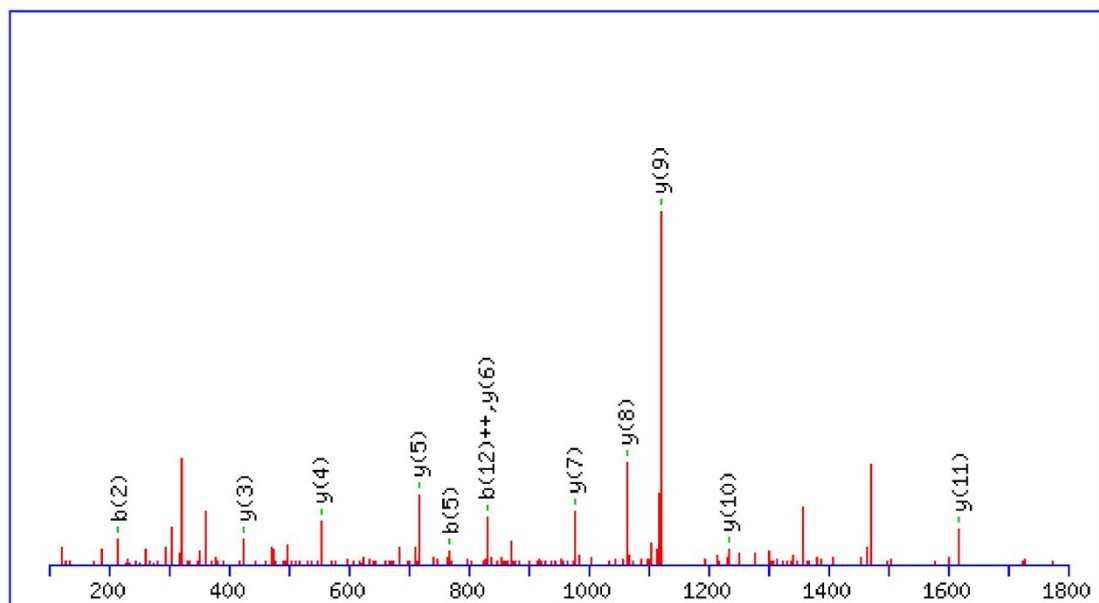
YLYEVAR



#	b	b ⁺⁺	b ⁰	b ⁰⁺⁺	Seq.	y	y ⁺⁺	y [*]	y ^{*++}	y ⁰	y ⁰⁺⁺	#
1	401.1496	201.0784			Y							7
2	514.2336	257.6205			L	750.4145	375.7109	733.3879	367.1976	732.4039	366.7056	6
3	677.2970	339.1521			Y	637.3304	319.1688	620.3039	310.6556	619.3198	310.1636	5
4	806.3396	403.6734	788.3290	394.6681	E	474.2671	237.6372	457.2405	229.1239	456.2565	228.6319	4
5	905.4080	453.2076	887.3974	444.2023	V	345.2245	173.1159	328.1979	164.6026			3
6	976.4451	488.7262	958.4345	479.7209	A	246.1561	123.5817	229.1295	115.0684			2
7					R	175.1190	88.0631	158.0924	79.5498			1

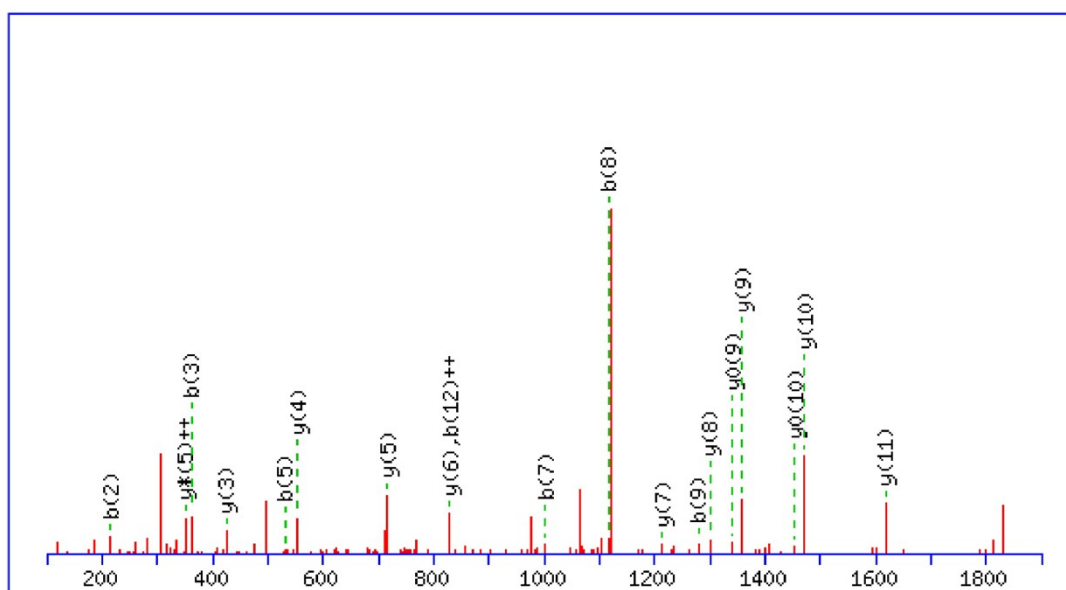
Phe 325

DVFLGSFLYEYSR



#	b	b ⁺⁺	b ⁰	b ⁰⁺⁺	Seq.	y	y ⁺⁺	y [*]	y ^{*++}	y ⁰	y ⁰⁺⁺	#
1	116.0342	58.5207	98.0237	49.5155	D							13
2	215.1026	108.0550	197.0921	99.0497	V	1717.8261	859.4167	1700.7995	850.9034	1699.8155	850.4114	12
3	599.2500	300.1287	581.2395	291.1234	F	1618.7577	809.8825	1601.7311	801.3692	1600.7471	800.8772	11
4	712.3341	356.6707	694.3235	347.6654	L	1234.6103	617.8088	1217.5837	609.2955	1216.5997	608.8035	10
5	769.3556	385.1814	751.3450	376.1761	G	1121.5262	561.2667	1104.4997	552.7535	1103.5156	552.2615	9
6	856.3876	428.6974	838.3770	419.6921	S	1064.5047	532.7560	1047.4782	524.2427	1046.4942	523.7507	8
7	1003.4560	502.2316	985.4454	493.2264	F	977.4727	489.2400	960.4462	480.7267	959.4621	480.2347	7
8	1116.5401	558.7737	1098.5295	549.7684	L	830.4043	415.7058	813.3777	407.1925	812.3937	406.7005	6
9	1279.6034	640.3053	1261.5928	631.3001	Y	717.3202	359.1638	700.2937	350.6505	699.3097	350.1585	5
10	1408.6460	704.8266	1390.6354	695.8213	E	554.2569	277.6321	537.2304	269.1188	536.2463	268.6268	4
11	1571.7093	786.3583	1553.6987	777.3530	Y	425.2143	213.1108	408.1878	204.5975	407.2037	204.1055	3
12	1658.7413	829.8743	1640.7308	820.8690	S	262.1510	131.5791	245.1244	123.0659	244.1404	122.5738	2
13					R	175.1190	88.0631	158.0924	79.5498			1

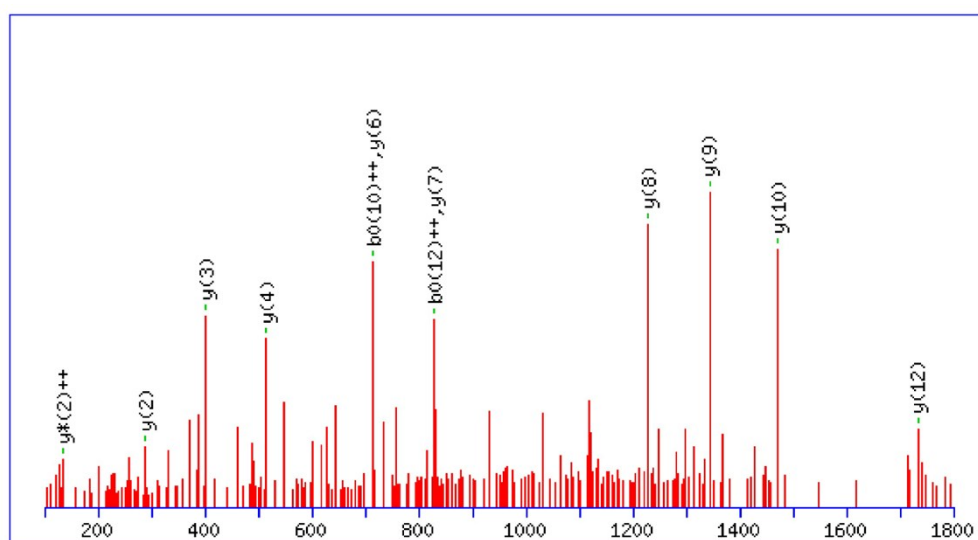
Phe 329

DVFLGSLY⁺EYSR

#	b	b ⁺⁺	b ⁰	b ⁰⁺⁺	Seq.	y	y ⁺⁺	y [*]	y ^{*++}	y ⁰	y ⁰⁺⁺	#
1	116.0342	58.5207	98.0237	49.5155	D							13
2	215.1026	108.0550	197.0921	99.0497	V	1717.8261	859.4167	1700.7995	850.9034	1699.8155	850.4114	12
3	362.1710	181.5892	344.1605	172.5839	F	1618.7577	809.8825	1601.7311	801.3692	1600.7471	800.8772	11
4	475.2551	238.1312	457.2445	229.1259	L	1471.6892	736.3483	1454.6627	727.8350	1453.6787	727.3430	10
5	532.2766	266.6419	514.2660	257.6366	G	1358.6052	679.8062	1341.5786	671.2930	1340.5946	670.8009	9
6	619.3086	310.1579	601.2980	301.1527	S	1301.5837	651.2955	1284.5572	642.7822	1283.5732	642.2902	8
7	1003.4560	502.2316	985.4454	493.2264	F	1214.5517	607.7795	1197.5251	599.2662	1196.5411	598.7742	7
8	1116.5401	558.7737	1098.5295	549.7684	L	830.4043	415.7058	813.3777	407.1925	812.3937	406.7005	6
9	1279.6034	640.3053	1261.5928	631.3001	Y	717.3202	359.1638	700.2937	350.6505	699.3097	350.1585	5
10	1408.6460	704.8266	1390.6354	695.8213	E	554.2569	277.6321	537.2304	269.1188	536.2463	268.6268	4
11	1571.7093	786.3583	1553.6987	777.3530	Y	425.2143	213.1108	408.1878	204.5975	407.2037	204.1055	3
12	1658.7413	829.8743	1640.7308	820.8690	S	262.1510	131.5791	245.1244	123.0659	244.1404	122.5738	2
13					R	175.1190	88.0631	158.0924	79.5498			1

Tyr 451

MPCTEDVLSLILNR



#	b	b ⁺⁺	b*	b ^{*++}	b ⁰	b ⁰⁺⁺	Seq.	y	y ⁺⁺	y*	y ^{*++}	y ⁰	y ⁰⁺⁺	#
1	132.0478	66.5275					M							14
2	229.1005	115.0539					P	1830.8731	915.9402	1813.8465	907.4269	1812.8625	906.9349	13
3	389.1312	195.0692					C	1733.8203	867.4138	1716.7938	858.9005	1715.8098	858.4085	12
4	490.1789	245.5931			472.1683	236.5878	T	1573.7897	787.3985	1556.7631	778.8852	1555.7791	778.3932	11
5	619.2214	310.1144			601.2109	301.1091	E	1472.7420	736.8746	1455.7155	728.3614	1454.7314	727.8694	10
6	734.2484	367.6278			716.2378	358.6225	D	1343.6994	672.3533	1326.6729	663.8401	1325.6888	663.3481	9
7	1134.3907	567.6990			1116.3801	558.6937	Y	1228.6725	614.8399	1211.6459	606.3266	1210.6619	605.8346	8
8	1247.4748	624.2410			1229.4642	615.2357	L	828.5302	414.7687	811.5036	406.2554	810.5196	405.7634	7
9	1334.5068	667.7570			1316.4962	658.7518	S	715.4461	358.2267	698.4195	349.7134	697.4355	349.2214	6
10	1447.5909	724.2991			1429.5803	715.2938	L	628.4141	314.7107	611.3875	306.1974			5
11	1560.6749	780.8411			1542.6644	771.8358	I	515.3300	258.1686	498.3035	249.6554			4
12	1673.7590	837.3831			1655.7484	828.3778	L	402.2459	201.6266	385.2194	193.1133			3
13	1787.8019	894.4046	1770.7754	885.8913	1769.7913	885.3993	N	289.1619	145.0846	272.1353	136.5713			2
14							R	175.1190	88.0631	158.0924	79.5498			1

RatSA MKWVTFLLLLFSGSAFSGRVFRREAHKSEIAHRFDLGEQHFKGLVLIATFSQYLQKCPYEEHKLKVOEVTDFAKTCVADENAENCDKSIHTLFGDKLCAIPKLRDNYGELADCCAKQEP
 RabSA MKWVTFISLLLFSSAYSARGVFRREAHKSEIAHRFNDVGEHFI GLVLIATFSQYLQKCPYEEHAKLVKEVTDLAKACVADESAENCDKSLHDIFGDKLCAIPSLRDTYGDVADCCCKKEP
 HSA MKWVTFISLLLFSSAYSARGVFRREDAHKSEVAHRFDLGEENFKALVLIATFAQYLQCCPFEDHVKLVNEVTEFAKTCVADESAENCDKSLHTLFGDKLCTVATLRETYGEMADCCAKQEP
 PorSA MKWVTFISLLLFSSAYSARGVFRRDYKSEIAHRFDLGEQYFKGLVLIATFSQHLQCCPYEEHVKLVRVTEFAKTCVADESAENCDKSIHTLFGDKLCAIPSLREHYGDLADCCCKKEP
 BSA MKWVTFISLLLFSSAYSARGVFRRDTHKSEIAHRFDLGEHFKGLVLIATFSQYLQCCPFDEHVKLVLNEVTEFAKTCVADESHAGCEKSLHTLFGDELCKVASLRETYGDMADCCCKQEP
 ShSA MKWVTFISLLLFSSAYSARGVFRRDTHKSEIAHRFNDLGEENFOGLVLIATFSQYLQCCPFDEHVKLVLNEVTEFAKTCVADESHAGCEKSLHTLFGDELCKVATLRETYGDMADCCCKQEP
 ***** :*: :*

 RatSA NAENCDKSIHTLFGDKLCAIPKLRDNYGELADCCAKQEPERNECFLOHKDDNPDLPPFQPEAEAMCTSFQENPTSLGHYLHEVARRHPYFYAPELLYAEKYNEVLTQCTTESDKAAC
 RabSA SAENCDKSLHDIFGDKLCAIPSLRDTYGDVADCCCKKEPERNECFLOHKDDNPDLPPFARPEADVLCKAFHDEKAFFGHYLYEVARRHPYFYAPELLYAQKYKAILTECCEAADKGAC
 HSA SAENCDKSLHTLFGDKLCTVATLRETYGEMADCCAKQEPERNECFLOHKDDNPDLPPFVRPEVDVMCTAFHDENEETELKKYLYETARRHPYFYAPELLYAKRYKAAFTCCQAADKAAC
 PorSA SAENCDKSIHTLFGDKLCAIPSLREHYGDLADCCCKKEPERNECFLOHKDDNPDLPPKLP-KPDPVALCADFQDEQKFWGKYLYETARRHPYFYAPELLYAIYKDVESCECQAADKAAC
 BSA SHAGCEKSLHTLFGDELCKVASLRETYGDMADCCCKQEPERNECFLOHKDDNPDLPPKLP-KPDPNTLCEFADEKKFWGKYLYETARRHPYFYAPELLYANKYNGVFOCCECQAADKGAC
 ShSA SHAGCEKSLHTLFGDELCKVATLRETYGDMADCCCKQEPERNECFLOHKDDNPDLPPKLP-KPEPDTLCAEFKADEKKFWGKYLYEVARRHPYFYAPELLYANKYNGVFOCCECQAADKGAC
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 RatSA LTPKLDLAVKEMALVAARVQRMKSSMQRFGERAFKAWAVARMSQRFPAEFAEITKLATDVTIKINKECCHGDLLECADDRADLAKYMCENQATISSKLQACCDKPVLEKSKCLAEIEHDN
 RabSA LTPKLDLAEGLSLISAAQERLRCAISIQFGDRAYKAWALVRLSQRFPKADFTDISKIVTDLTKVHKECCHGDLLECADDRADLAKYMECHQETISSHLKCCCDKPILEKAHCITYGLHNDE
 HSA LTPKLDLAEGLSLISAAQERLRCAISIQFGDRAYKAWAVARLSQRFPKAEFAEVSKLVTDLTKVHTECCHGDLLECADDRADLAKYICENQDSTISSKLKCCCKPILLEKSHCIAEVENDE
 PorSA LTPKIEHLREKVLTSAAKQRLKCAISIQFGDRAYKAWSLARLSQRFPKADFTDISKIVTDLAKVHKECCHGDLLECADDRADLAKYICENQDSTISSKLKCCCKPILLEKSHCIAEAKRDE
 BSA LTPKIEHTMREKVLTSAAQRLKCAISIQFGDRAYKAWSVARLSQKFPKAEFEVTKLIVTDLTKVHKECCHGDLLECADDRADLAKYICENQDSTISSKLKCCCKPILLEKSHCIAEVEKDA
 ShSA LTPKIDAMREKVLTSAAQRLKCAISIQFGDRAYKAWSVARLSQKFPKADFTDVTIKIVTDLTKVHKECCHGDLLECADDRADLAKYICDHQDALSSKLKCCCDKPVLEKSHCIAEVDKDA
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 RatSA IPEADLPSIAADFVEDKVECKNYAEAKDVFLGTFLYEYSRRHPDYSVLLRLAKKYEATLEKCCAEKGGPACGYGVLAEEFQPLVEEPKNLVKNCELYEKLGEYGFQNAVLYRYTKKAPQ
 RabSA TPACLPAAAEFVEDKDVCKNYEAKDLPLGKFLYEYSRRHPDYSVLLRLGKAYEATLEKCCATDDPHACYAKVLDEFFQPLVDEPKNLVKNCELYEKLGEYGFQNAVLYRYTKKVPQ
 HSA MEADLPSIAADFVEDKVECKNYAEAKDVFLGTFLYEYSRRHPDYSVLLRLAKTYETLEKCCAAADPHACYAKVDFEFKPLVEEPQNLVKNCELYEKLGEYGFQNAVLYRYTKKVPQ
 PorSA LPEADLNPLEHDFVEDKVECKNYEAKDVFLGTFLYEYSRRHPDYSVLLRLAKIYEATLEKCCAEKGGPACGYGVLAEEFQPLVDEPKNLVKNCELYEKLGEYGFQNAVLYRYTKKVPQ
 BSA IPENLPPITADFAEDKVECKNYEAKDVFLGSLYEYSRRHPDYSVLLRLAKEYEATLEKCCAEKGGPACGYGVLAEEFQPLVDEPKNLVKNCELYEKLGEYGFQNAVLYRYTKKVPQ
 ShSA VEENLPPITADFAEDKVECKNYEAKDVFLGSLYEYSRRHPDYSVLLRLAKEYEATLEKCCAEKGGPACGYGVLAEEFQPLVDEPKNLVKNCELYEKLGEYGFQNAVLYRYTKKAPQ
 * :*: :*

 RatSA VSTPTLVEAARNLGRVGTCTLPEAQRLPCVEDYLSAILNRLCVLHEKTPVSEKVTKCCSGSLVRRPCFSALTVDETYVPKEFKAETFTFHADICTLPDEKQIKKQATLALVELKHKP
 RabSA VSTPTLVEISRLGKVGSKCKKHEAERLPCVEDYLSVILNRLCVLHEKTPVSEKVTKCCSESLVDRRPCFSALGPDETYVPKEFNAETFTFHADICTLPETERKIKKQATLALVELKHKP
 HSA VSTPTLVEVSRNLGKVGSKCKKHEAKRMPCAEDYLSVILNRLCVLHEKTPVSEKVTKCCSESLVDRRPCFSALTVDETYVPKEFNAETFTFHADICTLPETERKIKKQATLALVELKHKP
 PorSA VSTPTLVEVARKLGLVGRCCRPEERLSCAEDYLSVILNRLCVLHEKTPVSEKVTKCCSESLVDRRPCFSALTVDETYVPKEFVEGFTFHADICTLPDEKQIKKQATLALVELKHKP
 BSA VSTPTLVEVSRNLGKVGTRCCTKPESERMPCEDYLSVILNRLCVLHEKTPVSEKVTKCCSESLVDRRPCFSALTVDETYVPKEFDEKLTFTFHADICTLPDEKQIKKQATLALVELKHKP
 ShSA VSTPTLVEISRLGKVGSKCAKPESERMPCEDYLSVILNRLCVLHEKTPVSEKVTKCCSESLVDRRPCFSALTVDETYVPKEFDEKLTFTFHADICTLPDEKQIKKQATLALVELKHKP
 ***** :*: :*

 RatSA KATPDQLTKVMGDFQFVDKCCAADKDNCFATEGNLVARSKAALA-
 RabSA HATNDQLTKTVVGEFTALLDKCSAEDKEACFAVEGPKLVESSKATLG-
 HSA KATKEQLKAVMDDFAAFVEKCCAKDDKCTCFAEFGKLVAAASQAALGL
 PorSA HATPEQLRTVLGNFAAFVQKCCAAPDHEACFAVEGPKFVIEIRGILA-
 BSA KATPEQLTKVMENFVAFVDKCCAADKDEACFAVEGPKLVVSTQTALA-
 ShSA KATPEQLTKVMENFVAFVDKCCAADKDEGCFVLEGGPKLVASTQAALA-

Figure S2. Multiple sequence alignment. Amino acid sequence alignments for *rat* (*RtSA*), *rabbit* (*RbSA*), *human* (*HSA*), *porcine* (*PSA*), *bovine* (*BSA*) and *sheep* (*SSA*) serum albumin proteins. Protein sequences were aligned using the CLUSTALW2 multiple sequence alignment (<https://www.ebi.ac.uk/Tools/msa/clustalw2/>). Fully conserved (*, blue, grey background) and functionally conserved (:, orange background) residues are highlighted.

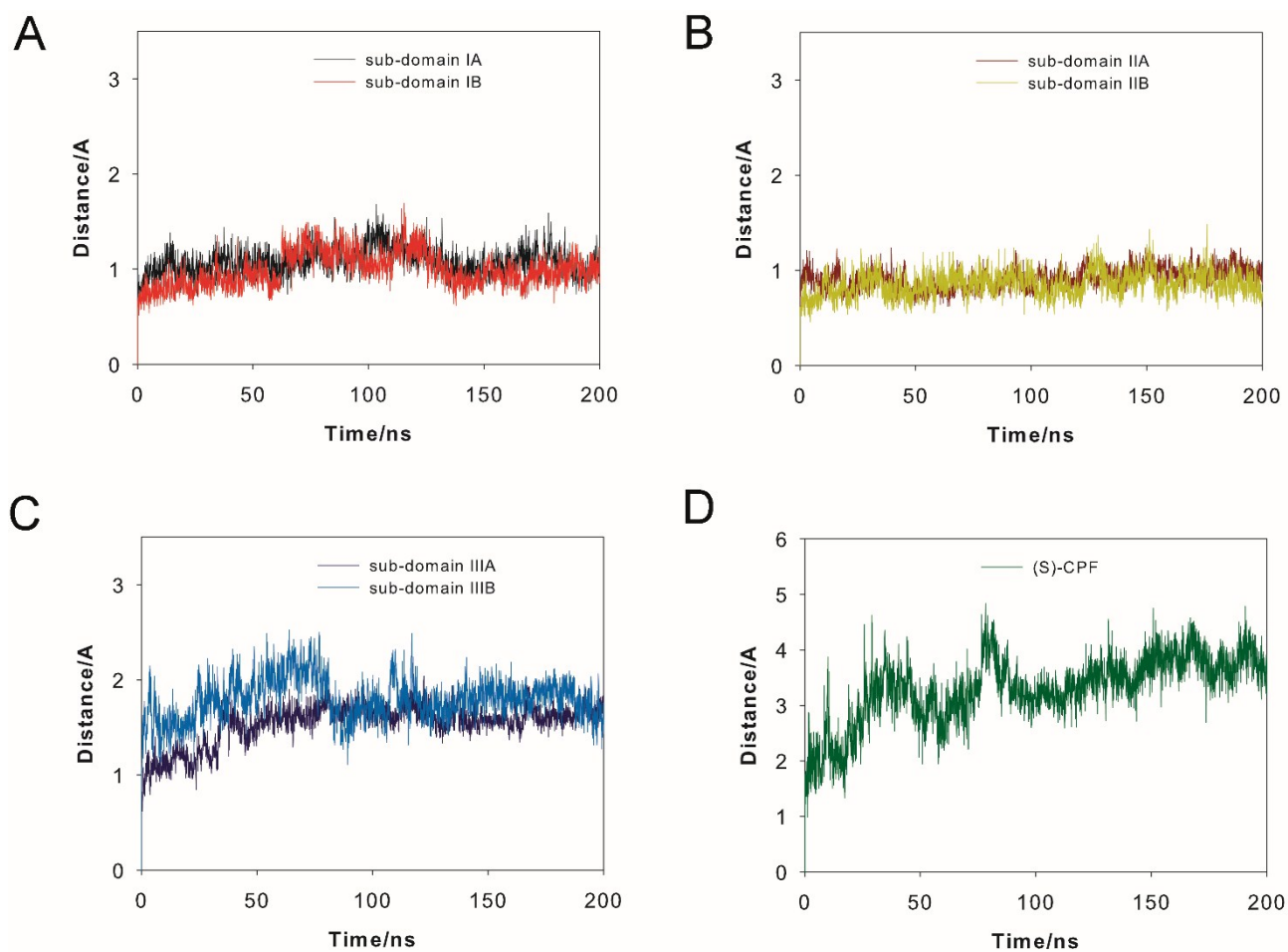


Figure S3. The rmsd plots for the three domains protein backbone ($C\alpha$, C, N and O atoms) and ligand calculated for the binary CPF/HSA-V cleft complex obtained from MD simulation studies: (A) domain I; (B) domain II; (C) domain III; and (D) CPF. Note how the complex is stable during the simulation as no significant changes are observed during the 200 ns of simulation.

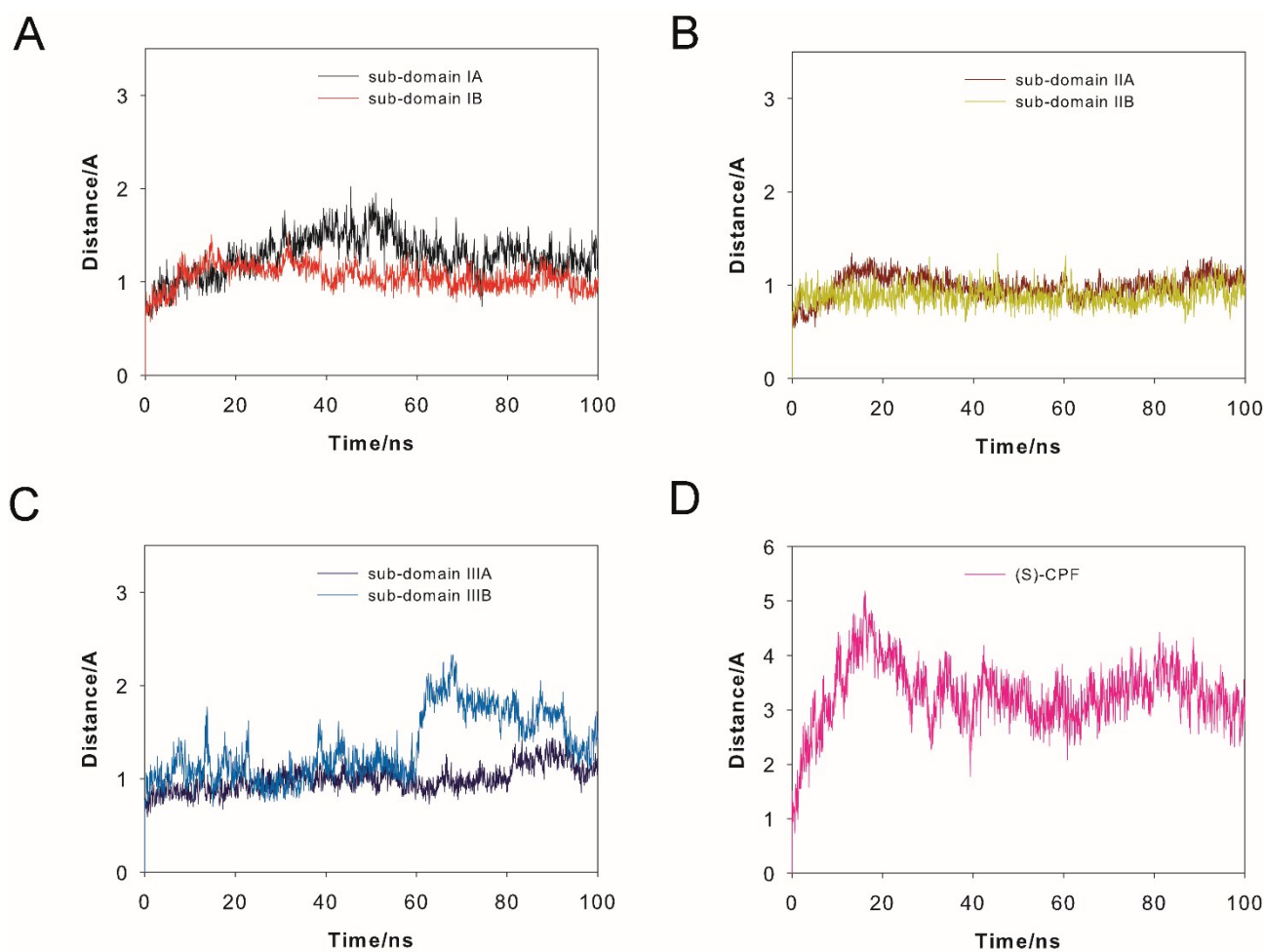


Figure S4. The rmsd plots for the three domains protein backbone ($C\alpha$, C, N and O atoms) and ligand calculated for the binary CPF/HSA-IB complex obtained from MD simulation studies: (A) domain I; (B) domain II; (C) domain III; and (D) CPF.