

## Supplementary information for manuscript

### “Deducing disulfide patterns of cysteine-rich proteins using signature fragments produced by top-down mass spectrometry”

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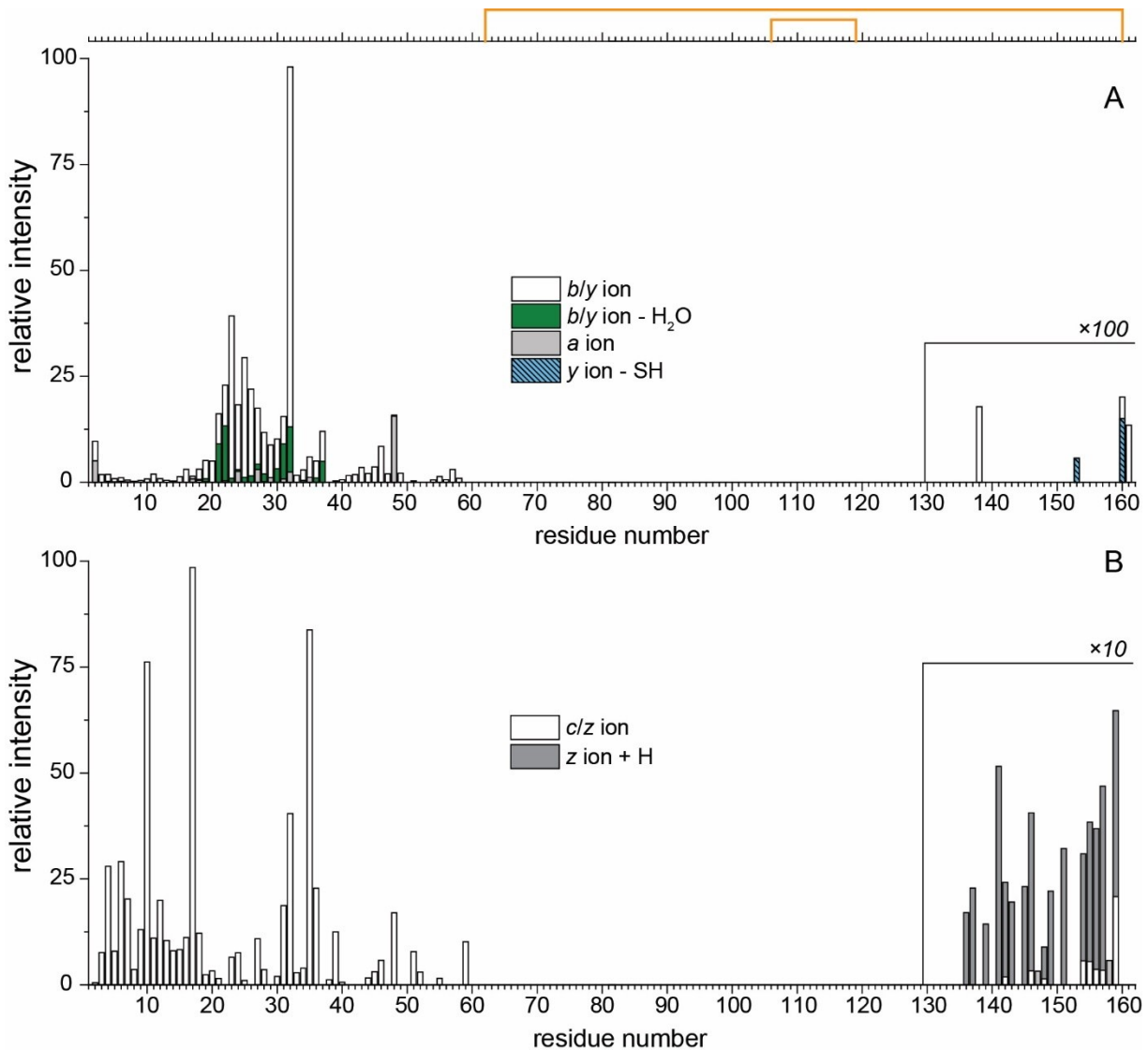
# *Equal contribution to this work.*

## 2 Supplementary Figures

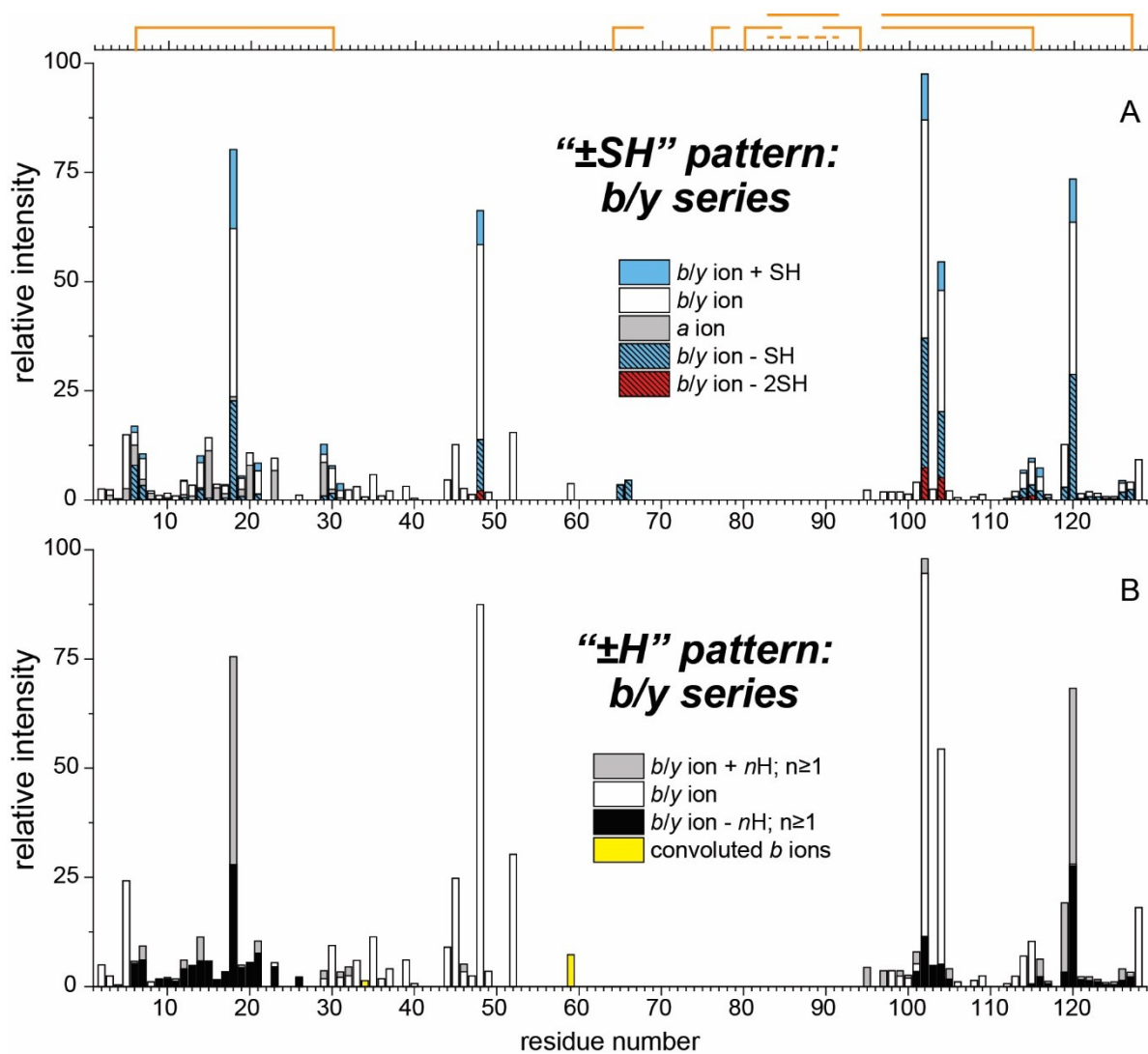
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**Fig. S1** Sequence coverage derived from top-down analysis of  $[\beta\text{-Lg}]^{16+}$ , and relative abundances of various fragments. **A:** abundances of *a*-, *b*- and *y*-type fragments, and the  $-\text{H}_2\text{O}$  and  $-\text{SH}$  modifications. **B:** abundances of *c*- and *z*-type fragments, and the  $+\text{H}$  modification. A schematic presentation of the disulfide pattern of  $\beta\text{-Lg}$  is shown on top.



**Fig. S2** Analysis of disulfide pattern of heat-stressed Lyz (incubated at 80 °C for 1 h). **A:** ±SH modification pattern of *a*-, *b*- and *y*-type fragments. **B:** ±H modification pattern of *b*- and *y*-type fragments. [Lyz]<sup>8+</sup> was mass-selected for EThcD. A schematic presentation of Cys-bridging relationships determined using the characteristic signature modifications is shown on top.

**Tab. S1** Fragment ions identified in measurements of native Lyz.

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
b2	1		228.1710	228.1702	-0.0008	228.1704	-0.0006	-2	135000
b3	1		375.2390	375.2383	-0.0007	375.2388	-0.0002	0	59850
b4	1		432.2610	432.2598	-0.0012	432.2605	-0.0005	-1	22300
b5	1		588.3620	588.3611	-0.0009	588.3621	0.0001	0	362650
b6	1	-H	689.3551	689.3549	-0.0002	689.3561	0.0010	1	68200
	1		690.3630	690.3583	-0.0047	690.3595	-0.0035	-5	22300
	1	+H	691.3709	691.3702	-0.0007	691.3714	0.0005	1	31660
	1	-SH	657.3830	657.3827	-0.0003	657.3838	0.0008	1	170980
	1	+SH	723.3430	723.3426	-0.0004	723.3439	0.0008	1	44650
b7	1	-H	818.3981	818.397	-0.0011	818.3985	0.0004	0	75100
	1		819.4060	819.4001	-0.0059	819.4016	-0.0044	-5	23100
	1	+H	820.4139	820.4131	-0.0008	820.4146	0.0006	1	107600
	1	-SH	786.4260	786.4252	-0.0008	786.4266	0.0006	1	68000
	1	+SH	852.3860	852.3849	-0.0011	852.3864	0.0004	0	41100
b8	1	-H	931.4821	931.4807	-0.0014	931.4824	0.0003	0	41100
	1		932.4900	932.4845	-0.0055	932.4862	-0.0038	-4	16100
	1	+H	933.4979	933.4971	-0.0008	933.4988	0.0008	1	9980
b9	1	-H	1002.5191	1002.5177	-0.0014	1002.5195	0.0005	0	79200
	1		1003.5270	1003.5214	-0.0056	1003.5232	-0.0038	-4	42100
	1	+H	1004.5349	1004.5355	0.0006	1004.5373	0.0024	2	5730
b10	1	-H	1073.5561	1073.5544	-0.0017	1073.5564	0.0003	0	94800
	1		1074.5640	1074.5582	-0.0058	1074.5602	-0.0038	-4	41200
	1	+H	1075.5719	1075.5712	-0.0007	1075.5732	0.0012	1	6620
b11	1	-H	1144.5931	1144.5916	-0.0015	1144.5937	0.0007	1	39700
	1		1145.6010	1145.5961	-0.0049	1145.5982	-0.0028	-2	18500
	1	+H	1146.6089	1146.6068	-0.0021	1146.6089	0.0000	0	12280
	2	+H	573.8084	573.8076	-0.0008	573.8086	0.0001	0	5760
b12	1	-H	1275.6331	1275.632	-0.0011	1275.6344	0.0013	1	85100
	1		1276.6410	1276.6361	-0.0049	1276.6385	-0.0025	-2	56600
	1	+H	1277.6489	1277.6471	-0.0018	1277.6495	0.0006	0	46800
	1	-SH	1243.6610	1243.6603	-0.0007	1243.6626	0.0016	1	29150
b13	2	-H	702.3680	702.3646	-0.0034	702.3658	-0.0022	-3	11800
	2		702.8720	702.8662	-0.0058	702.8674	-0.0046	-6	7730
	2	+H	703.3759	703.3752	-0.0007	703.3764	0.0005	1	11300
b14	2	-H	780.4190	780.4178	-0.0012	780.4192	0.0002	0	53900
	2		780.9230	780.92	-0.0030	780.9214	-0.0016	-2	42700
	2	+H	781.4269	781.4262	-0.0007	781.4276	0.0006	1	122030
	2	-SH	764.4330	764.4321	-0.0009	764.4334	0.0005	1	56550
	2	+SH	797.4130	797.4123	-0.0007	797.4137	0.0007	1	60160

**Tab. S1 Cont.**

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
b15	2	-H	848.9480	848.9476	-0.0004	848.9491	0.0011	1	108000
	2		849.4520	849.4493	-0.0027	849.4508	-0.0012	-1	96000
	2	+H	849.9559	849.9503	-0.0056	849.9518	-0.0041	-5	36900
	2	-SH	832.9620	832.9616	-0.0004	832.9631	0.0011	1	12560
	2	+SH	865.9420	865.9415	-0.0005	865.9431	0.0011	1	14920
b16	2	-H	877.4590	877.458	-0.0010	877.4596	0.0006	1	26600
	2		877.9630	877.9594	-0.0036	877.9610	-0.0020	-2	23600
	2	+H	878.4669	878.4623	-0.0046	878.4639	-0.0031	-3	9020
b17	2	-H	934.0010	934	-0.0010	934.0017	0.0007	1	45800
	2		934.5050	934.5014	-0.0036	934.5031	-0.0019	-2	45900
	2	+H	935.0089	935.0036	-0.0053	935.0053	-0.0036	-4	35740
	2	+SH	950.9950	950.9941	-0.0009	950.9958	0.0008	1	29050
b18	2	-H	991.5145	991.513	-0.0015	991.5148	0.0003	0	254000
	2		992.0185	992.0153	-0.0032	992.0171	-0.0014	-1	302000
	2	+H	992.5224	992.521	-0.0014	992.5228	0.0004	0	1704300
	2	-SH	975.5285	975.527	-0.0015	975.5288	0.0003	0	701200
	2	+SH	1008.5085	1008.507	-0.0015	1008.5088	0.0004	0	943480
b19	2	-H	1048.5360	1048.5348	-0.0012	1048.5367	0.0007	1	52100
	2		1049.0400	1049.0365	-0.0035	1049.0384	-0.0015	-1	52400
	2	+H	1049.5439	1049.5409	-0.0030	1049.5428	-0.0011	-1	86930
	2	-SH	1032.5500	1032.5498	-0.0002	1032.5517	0.0017	2	26930
	2	+SH	1065.5300	1065.5292	-0.0008	1065.5312	0.0012	1	33770
b20	2	-H	1130.0675	1130.068	0.0005	1130.0701	0.0026	2	63000
	2		1130.5715	1130.5675	-0.0040	1130.5696	-0.0019	-2	70100
	2	+H	1131.0754	1131.0684	-0.0070	1131.0705	-0.0049	-4	89800
b21	2	-H	1208.1180	1208.1168	-0.0012	1208.1191	0.0011	1	80700
	2		1208.6220	1208.6173	-0.0047	1208.6196	-0.0024	-2	88900
	2	+H	1209.1259	1209.1182	-0.0077	1209.1205	-0.0055	-5	121400
	3	-H	805.7480	805.7474	-0.0006	805.7488	0.0008	1	15800
	3		806.0840	806.0817	-0.0023	806.0831	-0.0008	-1	25700
	3	+H	806.4199	806.4171	-0.0028	806.4185	-0.0014	-2	127310
	3	-SH	795.0906	795.0902	-0.0004	795.0916	0.0010	1	51870
3	+SH	817.0773	817.076	-0.0013	817.0775	0.0002	0	73070	
b22	3		825.0913	825.0883	-0.0030	825.0898	-0.0015	-2	5170
	3	+H	825.4273	825.4253	-0.0020	825.4268	-0.0005	-1	10590
b23	2	-H	1318.1605	1318.1577	-0.0028	1318.1602	-0.0003	0	65300
	2		1318.6645	1318.6575	-0.0070	1318.6600	-0.0045	-3	77500
	2	+H	1319.1684	1319.1578	-0.0106	1319.1603	-0.0082	-6	96400
	3	-H	879.1096	879.108	-0.0016	879.1096	-0.0001	0	5320

**Tab. S1 Cont.**

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
b23	3		879.4456	879.443	-0.0026	879.4446	-0.0010	-1	11900
	3	+H	879.7816	879.7792	-0.0024	879.7808	-0.0008	-1	8600
b24	2	-H	1361.6765	1361.6746	-0.0019	1361.6772	0.0007	0	13500
	2		1362.1805	1362.1766	-0.0039	1362.1792	-0.0013	-1	20200
	2	+H	1362.6844	1362.6765	-0.0079	1362.6791	-0.0054	-4	12680
b25	2	-H	1418.2185	1418.2166	-0.0019	1418.2193	0.0008	1	12200
	2		1418.7225	1418.7189	-0.0036	1418.7216	-0.0009	-1	14300
	2	+H	1419.2264	1419.2192	-0.0072	1419.2219	-0.0046	-3	24950
b26	2	-H	1446.7295	1446.7292	-0.0003	1446.7319	0.0024	2	16900
	2		1447.2335	1447.2279	-0.0056	1447.2306	-0.0028	-2	27900
	2	+H	1447.7374	1447.731	-0.0064	1447.7337	-0.0037	-3	45930
b27	2	-H	1503.7510	1503.7499	-0.0011	1503.7528	0.0018	1	11700
	2		1504.2550	1504.2513	-0.0037	1504.2542	-0.0008	-1	11100
	2	+H	1504.7589	1504.7524	-0.0065	1504.7553	-0.0037	-2	96530
	2	+SH	1520.7450	1520.7432	-0.0018	1520.7461	0.0011	1	22240
	3		1003.1726	1003.1711	-0.0015	1003.1729	0.0003	0	5650
	3	+H	1003.5086	1003.5057	-0.0029	1003.5075	-0.0011	-1	38740
	3	-SH	1014.1660	1014.1652	-0.0008	1014.1671	0.0011	1	21890
b29	3	-H	1097.8856	1097.884	-0.0016	1097.8860	0.0004	0	2710
	3		1098.2216	1098.2177	-0.0039	1098.2197	-0.0019	-2	5630
	3	+H	1098.5576	1098.5557	-0.0019	1098.5577	0.0001	0	38990
	3	+SH	1109.5509	1109.5475	-0.0034	1109.5496	-0.0014	-1	17550
b30	3		1132.2223	1132.2217	-0.0006	1132.2238	0.0015	1	8760
	3	+H	1132.5583	1132.5563	-0.0020	1132.5584	0.0001	0	61260
	3	-SH	1121.2290	1121.2267	-0.0023	1121.2288	-0.0002	0	33900
b32	3	+H	1179.9163	1179.9122	-0.0041	1179.9144	-0.0019	-2	96860
b33	3	+H	1222.6146	1222.6133	-0.0013	1222.6156	0.0010	1	39400
b35	3		1314.3156	1314.3137	-0.0019	1314.3162	0.0005	0	9170
	3	+H	1314.6516	1314.6488	-0.0028	1314.6513	-0.0003	0	108760
	3	-SH	1303.9942	1303.9916	-0.0026	1303.9940	-0.0002	0	63280
b39	3	+SH	1325.3090	1325.3083	-0.0007	1325.3108	0.0018	1	47085
	3		1468.3776	1468.3754	-0.0022	1468.3782	0.0006	0	7860
	3	+H	1468.7136	1468.7119	-0.0017	1468.7147	0.0011	1	100800
b40	3	+SH	1479.7069	1479.7065	-0.0004	1479.7093	0.0024	2	29540
	3	+H	1502.3963	1502.3947	-0.0016	1502.3976	0.0013	1	27270
b41	3	+H	1545.0823	1545.0752	-0.0071	1545.0781	-0.0041	-3	36980
b42	3		1568.4256	1568.4235	-0.0021	1568.4265	0.0009	1	113160
b43	3	+H	1602.4439	1602.4376	-0.0063	1602.4407	-0.0033	-2	36845
b44	3		1640.1223	1640.1223	0.0000	1640.1254	0.0031	2	97250

Tab. S1 Cont.

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
b45	3		1692.1560	1692.1564	0.0004	1692.1596	0.0037	2	172985
	4	+H	1269.6209	1269.6172	-0.0037	1269.6196	-0.0014	-1	23180
b46	3	+H	1730.5063	1730.5052	-0.0011	1730.5085	0.0023	1	380900
	3	-SH	1719.5129	1719.5122	-0.0007	1719.5155	0.0026	1	56200
	4		1297.8797	1297.8778	-0.0019	1297.8802	0.0005	0	270535
	4	-SH	1290.1387	1290.1371	-0.0016	1290.1395	0.0008	1	52910
	4	+SH	1306.3767	1306.3746	-0.0021	1306.3771	0.0004	0	54600
b47	4	+H	1323.3937	1323.3892	-0.0045	1323.3917	-0.0020	-2	23860
b48	4		1351.6465	1351.6412	-0.0053	1351.6437	-0.0027	-2	5910
	4		1351.8985	1351.8969	-0.0016	1351.8994	0.0010	1	23500
	4	+H	1352.1504	1352.1471	-0.0033	1352.1496	-0.0008	-1	60500
	4	-SH	1343.4015	1343.3986	-0.0029	1343.4011	-0.0003	0	468830
	4	+SH	1360.1435	1360.1404	-0.0031	1360.1430	-0.0005	0	364300
	4	-2SH	1335.6604	1335.658	-0.0024	1335.6605	0.0001	0	23625
	4	+2SH	1368.6404	1368.6353	-0.0051	1368.6379	-0.0026	-2	55290
b49	4		1366.1537	1366.1538	0.0001	1366.1564	0.0027	2	154580
b50	4	+H	1388.1637	1388.161	-0.0027	1388.1636	-0.0001	0	114170
b52	4	+H	1442.1824	1442.1786	-0.0038	1442.1813	-0.0011	-1	243900
	4	-SH	1433.9374	1433.9335	-0.0039	1433.9362	-0.0012	-1	172890
	4	+SH	1450.1755	1450.1714	-0.0041	1450.1741	-0.0013	-1	109560
b63	5	+H	1437.2935	1437.2949	0.0014	1437.2976	0.0041	3	164890
b65	5	+H	1480.7039	1480.701	-0.0029	1480.7038	-0.0001	0	54620
b66	5	+H	1503.9109	1503.907	-0.0039	1503.9099	-0.0011	-1	66020
y2	1		288.2030	288.2024	-0.0006	288.2028	-0.0002	-1	393500
y3	1	-H	389.1961	389.1959	-0.0002	389.1965	0.0004	1	38200
	1	+H	391.2119	391.2114	-0.0005	391.2120	0.0000	0	57200
	1	-SH	357.2240	357.2238	-0.0002	357.2243	0.0003	1	77800
y4	1	+H	448.2339	448.2330	-0.0009	448.2337	-0.0002	-1	51470
	1	-SH	414.2460	414.2452	-0.0008	414.2458	-0.0002	0	48950
	1	+SH	480.2060	480.2052	-0.0008	480.2060	-0.0001	0	7560
y5	1	+H	604.3349	604.3343	-0.0006	604.3353	0.0004	1	15400
	1	-SH	570.3470	570.3459	-0.0011	570.3468	-0.0001	0	4320
y7	1	+H	903.4979	903.4977	-0.0002	903.4993	0.0014	2	15420
	1	-SH	869.5100	869.5098	-0.0002	869.5114	0.0014	2	10800
y8	1	+H	974.5349	974.5348	-0.0001	974.5366	0.0016	2	38800
	1	-SH	940.5470	940.5468	-0.0002	940.5485	0.0015	2	16240
y9	1	+H	1102.5939	1102.5929	-0.0010	1102.5949	0.0010	1	5950
y10	1	-H	1199.6461	1199.6461	0.0000	1199.6483	0.0023	2	106000
	1		1200.6540	1200.6470	-0.0070	1200.6492	-0.0048	-4	96400

Tab. S1 Cont.

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
y10	1	+H	1201.6619	1201.6624	0.0005	1201.6646	0.0027	2	473000
	1	-SH	1167.6740	1167.6736	-0.0004	1167.6758	0.0018	2	440620
	2	-H	600.3270	600.3265	-0.0005	600.3275	0.0005	1	29600
	2		600.8310	600.8279	-0.0031	600.8289	-0.0021	-3	17800
	2	+H	601.3349	601.3346	-0.0003	601.3356	0.0007	1	76700
	2	-SH	584.3410	584.3403	-0.0007	584.3413	0.0003	1	107200
	2	+SH	617.3210	617.3202	-0.0008	617.3212	0.0003	0	12400
y11	1	-H	1314.6731	1314.6727	-0.0004	1314.6752	0.0021	2	17100
	1		1315.6810	1315.6776	-0.0034	1315.6801	-0.0009	-1	14200
	1	+H	1316.6889	1316.6880	-0.0009	1316.6905	0.0015	1	196700
	1	-SH	1282.7010	1282.7007	-0.0003	1282.7031	0.0021	2	60340
y12	1	+H	1417.7369	1417.7361	-0.0008	1417.7388	0.0018	1	14810
y13	1	+H	1474.7589	1474.7579	-0.0010	1474.7607	0.0018	1	38090
	1	-SH	1440.7710	1440.7673	-0.0037	1440.7700	-0.0010	-1	19290
y14	1	+H	1602.8529	1602.8505	-0.0024	1602.8536	0.0006	0	86980
	1	-SH	1568.8650	1568.8639	-0.0011	1568.8669	0.0019	1	52330
	2	-H	800.9225	800.9227	0.0002	800.9241	0.0016	2	18000
	2		801.4265	801.4240	-0.0025	801.4254	-0.0011	-1	8290
	2	+H	801.9304	801.9297	-0.0007	801.9311	0.0007	1	24200
	2	-SH	784.9365	784.9358	-0.0007	784.9372	0.0007	1	9810
y15	2	+H	853.4354	853.4337	-0.0017	853.4352	-0.0002	0	10700
y16	2		930.4780	930.4769	-0.0011	930.4786	0.0006	1	19500
	2	+H	930.9819	930.9790	-0.0029	930.9807	-0.0013	-1	20300
	2	-SH	913.9880	913.9845	-0.0035	913.9861	-0.0018	-2	34250
	2	+SH	946.4640	946.4634	-0.0006	946.4651	0.0011	1	7760
y17	2		987.4995	987.4967	-0.0028	987.4985	-0.0010	-1	18450
y18	2	+H	1066.0539	1066.0515	-0.0024	1066.0535	-0.0005	0	6800
y22	2	+H	1337.1859	1337.1840	-0.0019	1337.1865	0.0006	0	5830
y25	2		1494.7425	1494.7390	-0.0035	1494.7418	-0.0006	0	46040
y26	2	-H	1522.7490	1522.7460	-0.0030	1522.7489	-0.0001	0	15500
	2		1523.2530	1523.2520	-0.0010	1523.2549	0.0019	1	50600
	2	+H	1523.7569	1523.7531	-0.0038	1523.7560	-0.0009	-1	305020
	2	-SH	1506.7630	1506.7616	-0.0014	1506.7645	0.0015	1	154170
	2	+SH	1539.7430	1539.7390	-0.0040	1539.7419	-0.0010	-1	95200
y28	2	-H	1608.2815	1608.2788	-0.0027	1608.2819	0.0004	0	48700
	2		1608.7855	1608.7831	-0.0024	1608.7862	0.0007	0	263000
	2	+H	1609.7934	1609.7867	-0.0067	1609.7898	-0.0036	-2	402000
	2	-SH	1591.7915	1591.7916	0.0001	1591.7946	0.0031	2	998100
	2	+SH	1624.7715	1624.7687	-0.0028	1624.7718	0.0003	0	547450



Tab. S1 Cont.

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
y28	2	-2SH	1575.8055	1575.8015	-0.0040	1575.8045	-0.0010	-1	215300
	3		1072.8596	1072.8575	-0.0021	1072.8595	-0.0002	0	27400
	3	+H	1073.1956	1073.1919	-0.0037	1073.1939	-0.0017	-2	45800
	3	-SH	1061.5303	1061.5305	0.0002	1061.5325	0.0021	2	170620
	3	+SH	1083.5170	1083.5148	-0.0022	1083.5168	-0.0002	0	37680
	3	-2SH	1050.8730	1050.8722	-0.0008	1050.8741	0.0012	1	31590
y45	3	+H	1645.8099	1645.8055	-0.0044	1645.8087	-0.0013	-1	11000
y60	4	+H	1618.7979	1618.7981	0.0002	1618.8012	0.0033	2	76400
c2	1		245.1970	245.1967	-0.0003	245.1970	0.0000	0	243300
c3	1		392.2660	392.2648	-0.0012	392.2654	-0.0006	-2	1393000
c4	1		449.2870	449.2863	-0.0007	449.2870	0.0000	0	1378000
c5	1		605.3880	605.3876	-0.0004	605.3886	0.0006	1	1793780
c6	1	-H	706.3821	706.3812	-0.0009	706.3824	0.0004	1	23600
	1		707.3900	707.3885	-0.0015	707.3897	-0.0003	0	36700
	1	+H	708.3979	708.3968	-0.0011	708.3980	0.0001	0	217320
	1	-SH	674.4100	674.4089	-0.0011	674.4101	0.0001	0	70100
	1	+SH	740.3700	740.3691	-0.0009	740.3704	0.0004	1	45460
c7	1	-H	835.4241	835.4238	-0.0003	835.4253	0.0012	1	87300
	1		836.4320	836.4307	-0.0013	836.4322	0.0002	0	84900
	1	+H	837.4399	837.4392	-0.0007	837.4407	0.0008	1	593100
	1	-SH	803.4520	803.4515	-0.0005	803.4529	0.0009	1	145640
	1	+SH	869.4120	869.4116	-0.0004	869.4132	0.0011	1	138810
c8	1	-H	948.5081	948.5077	-0.0004	948.5094	0.0014	1	44800
	1		949.5160	949.5148	-0.0012	949.5165	0.0005	1	68600
	1	+H	950.5239	950.5230	-0.0009	950.5247	0.0008	1	355200
	1	-SH	916.5360	916.5355	-0.0005	916.5372	0.0012	1	80000
	1	+SH	982.4960	982.4951	-0.0009	982.4969	0.0009	1	107300
c9	1	-H	1019.5451	1019.5446	-0.0005	1019.5465	0.0014	1	106000
	1		1020.5530	1020.5518	-0.0012	1020.5537	0.0007	1	181000
	1	+H	1021.5609	1021.5601	-0.0008	1021.5620	0.0010	1	868500
	1	-SH	987.5730	987.5723	-0.0007	987.5741	0.0011	1	185200
	1	+SH	1053.5330	1053.5325	-0.0005	1053.5344	0.0014	1	159500
c10	1	-H	1090.5821	1090.5817	-0.0004	1090.5837	0.0017	2	108000
	1		1091.5900	1091.5883	-0.0017	1091.5903	0.0003	0	187000
	1	+H	1092.5979	1092.5968	-0.0011	1092.5988	0.0009	1	794000
	1	-SH	1058.6100	1058.6095	-0.0005	1058.6114	0.0015	1	179800
	1	+SH	1124.5700	1124.5690	-0.0010	1124.5711	0.0011	1	142650
c11	1	-H	1161.6201	1161.6187	-0.0014	1161.6209	0.0008	1	48900
	1		1162.6280	1162.6251	-0.0029	1162.6273	-0.0007	-1	82500

Tab. S1 Cont.

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
c11	1	+H	1163.6359	1163.6337	-0.0022	1163.6359	-0.0001	0	376400
	1	-SH	1129.6480	1129.6467	-0.0013	1129.6488	0.0008	1	75750
	1	+SH	1195.6080	1195.6060	-0.0020	1195.6082	0.0002	0	70830
c12	1	-H	1292.6601	1292.6588	-0.0013	1292.6612	0.0012	1	30300
	1		1293.6680	1293.6659	-0.0021	1293.6683	0.0003	0	166000
	1	+H	1294.6759	1294.6738	-0.0021	1294.6762	0.0003	0	847100
	1	-SH	1260.6880	1260.6868	-0.0012	1260.6892	0.0012	1	288700
	1	+SH	1326.6480	1326.6460	-0.0020	1326.6485	0.0005	0	51400
	1	-H	1420.7551	1420.7543	-0.0008	1420.7570	0.0019	1	33700
c13	1		1421.7630	1421.7595	-0.0035	1421.7622	-0.0008	-1	70200
	1	+H	1422.7709	1422.7687	-0.0022	1422.7714	0.0005	0	349350
	1	-SH	1388.7830	1388.7816	-0.0014	1388.7842	0.0012	1	60010
	1	+SH	1454.7430	1454.7405	-0.0025	1454.7433	0.0002	0	42600
	1	-H	788.9320	788.9311	-0.0009	788.9325	0.0005	1	24100
c14	2		789.4360	789.4346	-0.0014	789.4360	0.0000	0	44300
	2	+H	789.9399	789.9387	-0.0012	789.9401	0.0002	0	245520
	2	-SH	772.9460	772.9449	-0.0011	772.9463	0.0003	0	53880
	2	+SH	805.9260	805.9246	-0.0014	805.9260	0.0001	0	39880
	2	-H	857.4615	857.4602	-0.0013	857.4617	0.0002	0	99900
c15	2		857.9655	857.9630	-0.0025	857.9645	-0.0009	-1	118000
	2	+H	858.4694	858.4682	-0.0012	858.4697	0.0003	0	435900
	2	-SH	841.4755	841.4745	-0.0010	841.4760	0.0005	1	128470
	2	+SH	874.4555	874.4539	-0.0016	874.4555	0.0000	0	147430
	2	-H	885.9720	885.9714	-0.0006	885.9730	0.0010	1	23100
c16	2		886.4760	886.4709	-0.0051	886.4725	-0.0035	-4	313000
	2	+H	886.9799	886.9789	-0.0010	886.9805	0.0006	1	277650
	2	-SH	869.9860	869.9850	-0.0010	869.9866	0.0006	1	82300
	2	+SH	902.9660	902.9652	-0.0008	902.9668	0.0009	1	68000
	2	-H	942.5145	942.5127	-0.0018	942.5144	-0.0001	0	44300
c17	2		943.0185	943.0160	-0.0025	943.0177	-0.0008	-1	79200
	2	+H	943.5224	943.5208	-0.0016	943.5225	0.0001	0	572840
	2	-SH	926.5285	926.5274	-0.0011	926.5291	0.0006	1	127400
	2	+SH	959.5085	959.5068	-0.0017	959.5085	0.0001	0	169680
	2	-H	1000.0275	1000.0266	-0.0009	1000.0284	0.0009	1	68700
c18	2		1000.5315	1000.5292	-0.0023	1000.5310	-0.0004	0	122000
	2	+H	1001.0354	1001.0340	-0.0014	1001.0358	0.0004	0	963600
	2	-SH	984.0415	984.0405	-0.0010	984.0423	0.0008	1	215400
	2	+SH	1017.0215	1017.0203	-0.0012	1017.0222	0.0007	1	255860
	2	-H	1057.0490	1057.0494	0.0004	1057.0513	0.0023	2	22100

Tab. S1 Cont.

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
c19	2		1057.5530	1057.5514	-0.0016	1057.5533	0.0004	0	22300
	2	+H	1058.0569	1058.0570	0.0001	1058.0589	0.0020	2	388700
	2	-SH	1041.0630	1041.0630	0.0000	1041.0649	0.0019	2	101490
	2	+SH	1074.0430	1074.0421	-0.0009	1074.0441	0.0011	1	84600
c20	2	-H	1138.5810	1138.5793	-0.0017	1138.5814	0.0004	0	39600
	2		1139.0850	1139.0818	-0.0032	1139.0839	-0.0011	-1	78600
	2	+H	1139.5889	1139.5867	-0.0022	1139.5888	-0.0001	0	709500
	2	-SH	1122.5950	1122.5936	-0.0014	1122.5957	0.0007	1	153540
c21	2	+SH	1155.5750	1155.5725	-0.0025	1155.5746	-0.0003	0	201800
	2	-H	1216.6315	1216.6294	-0.0021	1216.6317	0.0002	0	70300
	2		1217.1355	1217.1321	-0.0034	1217.1344	-0.0011	-1	127000
	2	+H	1217.6394	1217.6368	-0.0026	1217.6391	-0.0004	0	1208600
c21	2	-SH	1200.6455	1200.6470	0.0015	1200.6492	0.0038	3	174900
	2	+SH	1233.1215	1233.1187	-0.0028	1233.1210	-0.0005	0	342200
	3	-H	811.4236	811.4224	-0.0012	811.4238	0.0002	0	5330
	3		811.7596	811.7584	-0.0012	811.7598	0.0002	0	14700
	3	+H	812.0956	812.0937	-0.0019	812.0951	-0.0005	-1	82060
	3	-SH	801.1023	801.0996	-0.0027	801.1010	-0.0013	-2	14700
	3	+SH	822.7530	822.7521	-0.0009	822.7536	0.0006	1	24210
	3		822.7530	822.7521	-0.0009	822.7536	0.0006	1	24210
c22	2	-H	1245.1420	1245.1414	-0.0006	1245.1437	0.0017	1	14900
	2		1245.6460	1245.6429	-0.0031	1245.6452	-0.0007	-1	39100
	2	+H	1246.1499	1246.1473	-0.0026	1246.1496	-0.0003	0	368800
	2	-SH	1229.1560	1229.1543	-0.0017	1229.1566	0.0006	1	91900
	2	+SH	1262.1360	1262.1344	-0.0016	1262.1368	0.0008	1	191600
c23	2	-H	1326.6740	1326.6730	-0.0010	1326.6755	0.0015	1	43600
	2		1327.1780	1327.1744	-0.0036	1327.1769	-0.0011	-1	94200
	2	+H	1327.6819	1327.6791	-0.0028	1327.6816	-0.0003	0	1118500
	2	-SH	1310.6880	1310.6863	-0.0017	1310.6888	0.0008	1	161550
	2	+SH	1343.6680	1343.6648	-0.0032	1343.6673	-0.0006	0	124000
	3		885.1213	885.1196	-0.0017	885.1212	-0.0001	0	12600
	3	+H	885.4573	885.4556	-0.0017	885.4572	-0.0001	0	147970
c23	3	+SH	896.1146	896.1107	-0.0039	896.1123	-0.0023	-3	10780
	2	-H	1370.1900	1370.1881	-0.0019	1370.1907	0.0007	1	8640
	2		1370.6940	1370.6903	-0.0037	1370.6929	-0.0011	-1	20500
	2	+H	1371.1979	1371.1948	-0.0031	1371.1974	-0.0006	0	344230
	2	-SH	1354.2040	1354.2020	-0.0020	1354.2046	0.0006	0	67950
	2	+SH	1387.1840	1387.1796	-0.0044	1387.1822	-0.0018	-1	102010
c24	3		914.4679	914.4661	-0.0018	914.4678	-0.0002	0	20650
	2	-H	1426.7320	1426.7311	-0.0009	1426.7338	0.0018	1	6350

Tab. S1 Cont.

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
c25	2		1427.2360	1427.2323	-0.0037	1427.2350	-0.0010	-1	23000
	2	+H	1427.7399	1427.7368	-0.0031	1427.7395	-0.0004	0	277000
	2	-SH	1410.7460	1410.7443	-0.0017	1410.7470	0.0010	1	41780
	2	+SH	1443.7260	1443.7228	-0.0032	1443.7255	-0.0004	0	61540
	3	-H	951.4906	951.4907	0.0001	951.4974	0.0018	2	50030
	3	+H	952.1626	952.1605	-0.0021	952.1622	-0.0004	0	38830
c26	2	-H	1455.2425	1455.2412	-0.0013	1455.2440	0.0015	1	15200
	2		1455.7465	1455.7439	-0.0026	1455.7467	0.0002	0	53500
	2	+H	1456.2504	1456.2477	-0.0027	1456.2505	0.0000	0	360980
	2	-SH	1439.2565	1439.2545	-0.0020	1439.2572	0.0008	1	51800
	2	+SH	1472.2365	1472.2344	-0.0021	1472.2372	0.0007	0	81500
	3	-H	970.4976	970.4907	-0.0069	970.4925	-0.0052	-5	8710
	3		970.8336	970.8327	-0.0009	970.8345	0.0008	1	8700
	3	+H	971.1696	971.1664	-0.0032	971.1682	-0.0014	-1	78700
c27	2		1512.7680	1512.7659	-0.0021	1512.7688	0.0008	1	5320
	2	+H	1513.2719	1513.2675	-0.0044	1513.2704	-0.0016	-1	110400
c28	3		1070.8743	1070.8723	-0.0020	1070.8743	0.0000	0	27830
	3	+H	1071.2103	1071.2065	-0.0038	1071.2085	-0.0018	-2	16430
c29	3		1103.8973	1103.8960	-0.0013	1103.8980	0.0007	1	8330
	3	+H	1104.2333	1104.2312	-0.0021	1104.2332	0.0000	0	160190
	3	+SH	1114.8906	1114.8895	-0.0011	1114.8916	0.0009	1	73550
c32	3	+H	1185.5916	1185.5879	-0.0037	1185.5901	-0.0015	-1	113470
	3	-SH	1174.5983	1174.5986	0.0003	1174.6008	0.0025	2	48800
c35	3	+H	1320.3269	1320.3241	-0.0028	1320.3266	-0.0004	0	138440
c36	3	-H	1348.6656	1348.6630	-0.0026	1348.6655	-0.0001	0	137520
	3		1349.0016	1348.9987	-0.0029	1349.0012	-0.0004	0	12800
	3	+H	1349.3376	1349.3342	-0.0034	1349.3367	-0.0009	-1	112820
	3	-SH	1337.6723	1337.6688	-0.0035	1337.6713	-0.0010	-1	136610
	3	+SH	1359.9950	1359.9915	-0.0035	1359.9941	-0.0009	-1	43600
	3	-2SH	1327.0150	1327.0122	-0.0028	1327.0147	-0.0003	0	20980
c37	3	+H	1387.3519	1387.3502	-0.0017	1387.3528	0.0009	1	22605
c38	4	+H	1436.3749	1436.3729	-0.0020	1436.3756	0.0007	0	65165
c39	4	+H	1474.3893	1474.3865	-0.0028	1474.3893	0.0000	0	137990
c44	3	+H	1646.1339	1646.1300	-0.0039	1646.1332	-0.0008	0	66470
	3	-SH	1635.4766	1635.4706	-0.0060	1635.4737	-0.0029	-2	12960
c45	3	+H	1698.1676	1698.1643	-0.0033	1698.1676	0.0000	0	269300
	3	-SH	1687.1743	1687.1709	-0.0034	1687.1741	-0.0001	0	86100
	4		1273.6257	1273.6244	-0.0013	1273.6268	0.0011	1	8130
	4	+H	1273.8777	1273.8746	-0.0031	1273.8770	-0.0007	-1	102570

Tab. S1 Cont.

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
c45	4	-SH	1265.6327	1265.6252	-0.0075	1265.6276	-0.0051	-3	40620
	4	+SH	1282.1227	1282.1176	-0.0051	1282.1200	-0.0027	-2	37310
c46	3	+H	1736.5179	1736.5161	-0.0018	1736.5194	0.0015	1	498200
	4	+H	1302.3884	1302.3868	-0.0016	1302.3892	0.0008	1	308390
	4	+SH	1310.3815	1310.3787	-0.0028	1310.3812	-0.0003	0	87510
c47	4	+H	1327.6502	1327.6490	-0.0012	1327.6515	0.0013	1	100725
	4	-SH	1319.6572	1319.6580	0.0008	1319.6605	0.0033	3	41470
c49	4	+H	1370.6624	1370.6630	0.0006	1370.6656	0.0031	2	206100
c50	4	+H	1392.4204	1392.4154	-0.0050	1392.4180	-0.0024	-2	184430
c51	4	+H	1417.6824	1417.6759	-0.0065	1417.6786	-0.0039	-3	31260
c63	5	+H	1440.6989	1440.6918	-0.0071	1440.6945	-0.0044	-3	192960
	5	+SH	1447.4965	1447.4916	-0.0049	1447.4943	-0.0022	-2	86130
z2	1		271.1760	271.1758	-0.0002	271.1761	0.0001	0	76000
z3	1	-H	372.1701	372.1693	-0.0008	372.1698	-0.0002	-1	14900
	1		373.1780	373.1771	-0.0009	373.1776	-0.0004	-1	80200
	1	+H	374.1859	374.1848	-0.0011	374.1853	-0.0006	-2	285000
	1	-SH	340.1980	340.1972	-0.0008	340.1977	-0.0003	-1	55900
	1	+SH	406.1580	406.1565	-0.0015	406.1571	-0.0009	-2	2810
	1		429.1911	429.1907	-0.0004	429.1914	0.0003	1	9500
z4	1		430.1990	430.1986	-0.0004	430.1993	0.0003	1	13300
	1	+H	431.2069	431.2063	-0.0006	431.2070	0.0000	0	120600
	1	-H	585.2921	585.2918	-0.0003	585.2928	0.0007	1	11700
z5	1	+H	587.3079	587.3077	-0.0002	587.3087	0.0007	1	88100
	1	-SH	553.3200	553.3195	-0.0005	553.3204	0.0004	1	2760
	1	+SH	619.2800	619.2795	-0.0005	619.2805	0.0005	1	13730
	1	-H	698.3761	698.3750	-0.0011	698.3762	0.0001	0	3210
z6	1		699.3840	699.3843	0.0003	699.3855	0.0015	2	2680
	1	+H	700.3919	700.3916	-0.0003	700.3928	0.0009	1	439100
	1	-SH	666.4040	666.4047	0.0007	666.4058	0.0019	3	2660
	1	-H	884.4561	884.4548	-0.0013	884.4564	0.0003	0	19700
z7	1	+H	886.4719	886.4709	-0.0010	886.4725	0.0006	1	423000
	1	-SH	852.4840	852.4831	-0.0009	852.4846	0.0006	1	30200
	1	+SH	918.4440	918.4420	-0.0020	918.4437	-0.0004	0	27310
	1	-H	955.4931	955.4920	-0.0011	955.4937	0.0007	1	13700
z8	1		956.5010	956.4990	-0.0020	956.5007	-0.0003	0	8980
	1	+H	957.5089	957.5080	-0.0009	957.5097	0.0008	1	1342300
	1	-SH	923.5210	923.5203	-0.0007	923.5220	0.0010	1	14280
	1	-H	1083.5511	1083.5472	-0.0039	1083.5492	-0.0019	-2	15000
z9	1		1084.5590	1084.5532	-0.0058	1084.5552	-0.0038	-4	5660

Tab. S1 Cont.

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
z9	1	+H	1085.5669	1085.5662	-0.0007	1085.5682	0.0013	1	193450
z10	1	-H	1182.6201	1182.6196	-0.0005	1182.6218	0.0017	1	27200
	1		1183.6280	1183.6237	-0.0043	1183.6259	-0.0021	-2	17000
	1	+H	1184.6359	1184.6348	-0.0011	1184.6370	0.0011	1	119350
	1	-SH	1150.6480	1150.6472	-0.0008	1150.6493	0.0013	1	50960
z11	1	-H	1297.6471	1297.6483	0.0012	1297.6507	0.0037	3	16300
	1		1298.6550	1298.6504	-0.0046	1298.6528	-0.0022	-2	7680
	1	+H	1299.6629	1299.6638	0.0009	1299.6662	0.0033	3	166400
	1	-SH	1265.6750	1265.6742	-0.0008	1265.6766	0.0016	1	66750
	2	+H	650.3354	650.3348	-0.0006	650.3359	0.0005	1	15320
z12	1	-H	1398.6951	1398.6941	-0.0010	1398.6967	0.0017	1	39300
	1		1399.7030	1399.6985	-0.0045	1399.7011	-0.0019	-1	37700
	1	+H	1400.7109	1400.7085	-0.0024	1400.7111	0.0002	0	919600
	1	-SH	1366.7230	1366.7218	-0.0012	1366.7244	0.0014	1	110400
	1	+SH	1432.6830	1432.6807	-0.0023	1432.6834	0.0004	0	31200
	2	+H	700.8594	700.8581	-0.0013	700.8593	-0.0001	0	91930
z13	2	+H	729.3699	729.3691	-0.0008	729.3704	0.0004	1	35350
z14	2	+H	793.9214	793.9185	-0.0029	793.9199	-0.0015	-2	10970
z15	1		1686.8200	1686.8187	-0.0013	1686.8219	0.0019	1	316000
	1	-SH	1652.8320	1652.8319	-0.0001	1652.8351	0.0030	2	78900
	1	-2SH	1620.8600	1620.8589	-0.0011	1620.8620	0.0020	1	173910
	2	+H	844.4179	844.4146	-0.0033	844.4161	-0.0018	-2	15750
z16	2	+H	922.4684	922.4662	-0.0022	922.4679	-0.0006	-1	52980
z17	2		978.9860	978.9853	-0.0007	978.9871	0.0011	1	13200
	2	+H	979.4899	979.4871	-0.0028	979.4889	-0.0011	-1	10500
z19	2		1150.0765	1150.0746	-0.0019	1150.0767	0.0003	0	32500
	2	+H	1150.5804	1150.5763	-0.0041	1150.5784	-0.0020	-2	41000
	2	-SH	1133.5865	1133.5834	-0.0031	1133.5855	-0.0010	-1	60850
	2	+SH	1166.0625	1166.0623	-0.0002	1166.0645	0.0020	2	14360
z20	2		1185.5950	1185.5908	-0.0042	1185.5930	-0.0020	-2	20100
	2	+H	1186.0989	1186.0944	-0.0045	1186.0966	-0.0023	-2	13200
z21	2	+H	1235.6329	1235.6295	-0.0034	1235.6318	-0.0011	-1	42200
	2	+SH	1251.6190	1251.6143	-0.0047	1251.6166	-0.0023	-2	58100
	2	-2SH	1202.1490	1202.1478	-0.0012	1202.1500	0.0011	1	59405
z23	2		1363.6875	1363.6871	-0.0004	1363.6897	0.0022	2	8260
	2	+H	1364.1914	1364.1884	-0.0030	1364.1910	-0.0005	0	18500
z24	2		1420.7090	1420.7087	-0.0003	1420.7114	0.0024	2	20300
	2	+H	1421.2129	1421.2097	-0.0032	1421.2124	-0.0005	0	29300
	2	-SH	1404.2190	1404.2200	0.0010	1404.2227	0.0037	3	111090

**Tab. S1 Cont.**

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
z24	2	+SH	1437.1990	1437.1952	-0.0038	1437.1979	-0.0011	-1	0
z25	2	+H	1486.7329	1486.7290	-0.0039	1486.7318	-0.0011	-1	111850
z26	2		1514.7400	1514.7373	-0.0027	1514.7402	0.0002	0	29600
	2	+H	1515.2439	1515.2395	-0.0044	1515.2424	-0.0016	-1	42100
	2	-SH	1498.2500	1498.2484	-0.0016	1498.2512	0.0013	1	269870
	2	+SH	1531.7339	1531.7257	-0.0082	1531.7286	-0.0053	-3	137400
	2	-2SH	1481.7600	1481.7612	0.0012	1481.7640	0.0041	3	47290
z27	2		1571.7615	1571.7584	-0.0031	1571.7614	-0.0001	0	30600
	2	+H	1572.2654	1572.2600	-0.0054	1572.2630	-0.0024	-2	36800
	2		1554.7675	1554.7631	-0.0044	1554.7661	-0.0014	-1	179600
	2	+SH	1588.2515	1588.2424	-0.0091	1588.2454	-0.0060	-3	74700
	2	-2SH	1539.7894	1539.7848	-0.0046	1539.7877	-0.0017	-1	14950
z28	2	-H	1599.7680	1599.7604	-0.0076	1599.7635	-0.0045	-3	17600
	2		1600.2720	1600.2699	-0.0021	1600.2730	0.0010	1	40100
	2	+H	1600.7759	1600.7728	-0.0031	1600.7759	-0.0001	0	73900
	2	+SH	1616.2580	1616.2593	0.0013	1616.2624	0.0044	3	158200
z29	2	+H	1658.2894	1658.2872	-0.0022	1658.2904	0.0009	1	182900
z41	3	+H	1506.0759	1506.0736	-0.0023	1506.0765	0.0005	0	56800
z61	4	+H	1640.0552	1640.0524	-0.0028	1640.0555	0.0004	0	49410
z63	4	+H	1693.0837	1693.0831	-0.0006	1693.0863	0.0027	2	107000

1. Recalibrated using the equation: recalibrated m/z = (measured m/z) - (measured m/z)\*k -b, where  $k=-2.05225*10^{-6}$ ,  $b=2.26612*10^{-4}$ , (determined by linear fitting of the (absolute error) vs. (measured m/z) data) ;

2. Error tolerance was set as  $\pm 3$  ppm for F $\pm$ SH ions and the smallest F+nH (n=-1, 0, 1) ions, and  $\pm 6$  ppm for F+(n+1)H (n=-1, 0, 1) ions, because the contribution of <sup>13</sup>C;

3. For F $\pm$ H species, additional deconvolution is needed to determine the abundances of F-H, F and F+H (see Results section for detail).

**Tab. S2** Fragment ions identified in measurements of disulfide-scrambled Lyz.

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
b2	1		228.1710	228.1711	0.0001	228.1704	-0.0006	-3	24730
b3	1		375.2390	375.2397	0.0007	375.2388	-0.0002	0	12020
b4	1		432.2610	432.2613	0.0003	432.2604	-0.0006	-1	1750
b5	1		588.3620	588.3629	0.0009	588.3618	-0.0002	0	120900
b6	1	-H	689.3551	689.3570	0.0019	689.3558	0.0008	1	17200
	1		690.3630	690.3611	-0.0019	690.3599	-0.0031	-4	5290
	1	+H	691.3709	691.3724	0.0015	691.3712	0.0003	0	4870
	1	-SH	657.3830	657.3846	0.0016	657.3835	0.0005	1	77910
	1	+SH	723.3430	723.3446	0.0016	723.3434	0.0004	1	14140
b7	1	-H	818.3981	818.3995	0.0014	818.3982	0.0002	0	4050
	1		819.4060	819.4049	-0.0011	819.4036	-0.0024	-3	1460
	1	+H	820.4139	820.4152	0.0013	820.4139	0.0000	0	24110
	1	-SH	786.4260	786.4260	0.0000	786.4247	-0.0012	-2	32500
	1	+SH	852.3860	852.3875	0.0015	852.3862	0.0002	0	10820
b8	1		933.4979	933.4998	0.0019	933.4984	0.0005	1	2580
	1	+H	899.5100	899.5119	0.0019	899.5105	0.0006	1	1320
b9	1	-H	1002.5191	1002.5210	0.0019	1002.5195	0.0005	0	4430
	1		1003.5270	1003.5238	-0.0032	1003.5223	-0.0047	-5	1660
	1	+H	1004.5349	1004.5369	0.0020	1004.5354	0.0005	1	2060
	1	-SH	970.5470	970.5490	0.0020	970.5476	0.0006	1	1120
b10	1	-H	1073.5561	1073.5583	0.0022	1073.5568	0.0007	1	4470
	1		1074.5640	1074.5631	-0.0009	1074.5616	-0.0024	-2	1990
	1	+H	1075.5719	1075.5742	0.0023	1075.5727	0.0007	1	3170
	1	-SH	1041.5840	1041.5859	0.0019	1041.5844	0.0004	0	1370
b11	1	-H	1144.5931	1144.5947	0.0016	1144.5931	0.0001	0	2950
	1		1145.6010	1145.6003	-0.0007	1145.5987	-0.0023	-2	1500
	1	+H	1146.6089	1146.6108	0.0019	1146.6092	0.0003	0	4120
b12	1	-H	1275.6331	1275.6362	0.0031	1275.6345	0.0014	1	8980
	1		1276.6410	1276.6401	-0.0009	1276.6384	-0.0026	-2	5940
	1	+H	1277.6489	1277.6528	0.0039	1277.6511	0.0022	2	15020
	1	-SH	1243.6610	1243.6642	0.0032	1243.6625	0.0015	1	5150
	1	+SH	1309.6210	1309.6224	0.0014	1309.6207	-0.0003	0	2000
b13	1	-H	1403.7281	1403.7340	0.0059	1403.7322	0.0041	3	24350
	1		1404.7360	1404.7313	-0.0047	1404.7295	-0.0065	-5	6520
	1	+H	1405.7439	1405.7476	0.0037	1405.7458	0.0018	1	7030
b14	1	-H	1559.8301	1559.8320	0.0019	1559.8300	0.0000	0	3540
	1		1560.8380	1560.8356	-0.0024	1560.8336	-0.0044	-3	3280
	1	+H	1561.8459	1561.8468	0.0009	1561.8448	-0.0011	-1	9490
	2	-H	780.4190	780.4200	0.0010	780.4188	-0.0002	0	7370



Tab. S2 Cont.

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
b14	2		780.9230	780.9219	-0.0011	780.9207	-0.0023	-3	6400
	1	+H	781.4269	781.4283	0.0014	781.4270	0.0001	0	26500
	2	-SH	764.4330	764.4340	0.0010	764.4328	-0.0002	0	23290
	2	+SH	797.4130	797.4140	0.0010	797.4127	-0.0002	0	15070
b15	2	-H	848.9480	848.9508	0.0028	848.9495	0.0015	2	29220
	2		849.4520	849.4525	0.0005	849.4512	-0.0008	-1	11900
	2	+H	849.9559	849.9544	-0.0015	849.9531	-0.0029	-3	4720
	2	-SH	832.9620	832.9640	0.0020	832.9627	0.0007	1	4070
b16	2	-H	877.4590	877.4604	0.0014	877.4591	0.0001	0	7980
	2		877.9630	877.9624	-0.0006	877.9611	-0.0019	-2	3060
	2	+H	878.4669	878.4642	-0.0027	878.4629	-0.0041	-5	1630
b17	2	-H	934.0010	934.0022	0.0012	934.0008	-0.0002	0	17170
	2		934.5050	934.5046	-0.0004	934.5032	-0.0018	-2	5370
	2	+H	935.0089	935.0089	0.0000	935.0075	-0.0014	-2	6410
	2	-SH	918.0150	918.0161	0.0011	918.0147	-0.0002	0	4145
	2	+SH	950.9950	950.9966	0.0016	950.9952	0.0002	0	2940
b18	2	-H	991.5145	991.5156	0.0011	991.5142	-0.0003	0	41900
	2		992.0185	992.0178	-0.0007	992.0164	-0.0021	-2	44300
	2	+H	992.5224	992.5237	0.0013	992.5223	-0.0002	0	290570
	2	-SH	975.5285	975.5294	0.0009	975.5280	-0.0005	-1	222640
	2	+SH	1008.5085	1008.5095	0.0010	1008.5080	-0.0004	0	177470
b19	2	-H	1048.5360	1048.5377	0.0017	1048.5362	0.0002	0	6250
	2		1049.0400	1049.0406	0.0006	1049.0391	-0.0009	-1	5830
	2	+H	1049.5439	1049.5439	0.0000	1049.5424	-0.0015	-1	11380
	2	-SH	1032.5500	1032.5515	0.0015	1032.5500	0.0001	0	8000
	2	+SH	1065.5300	1065.5321	0.0021	1065.5306	0.0006	1	4980
b20	2	-H	1130.0675	1130.0695	0.0020	1130.0679	0.0004	0	27650
	2		1130.5715	1130.5708	-0.0007	1130.5692	-0.0022	-2	8350
	2	+H	1131.0754	1131.0717	-0.0037	1131.0701	-0.0053	-5	11500
b21	2	-H	1208.1180	1208.1210	0.0030	1208.1194	0.0014	1	27280
	2		1208.6220	1208.6205	-0.0015	1208.6189	-0.0031	-3	5980
	2	+H	1209.1259	1209.1232	-0.0027	1209.1216	-0.0044	-4	14340
	2	+SH	1225.1120	1225.1156	0.0036	1225.1139	0.0020	2	6270
	3	-H	805.7480	805.7490	0.0010	805.7477	-0.0003	0	2590
	3		806.0840	806.0845	0.0005	806.0832	-0.0007	-1	3070
	3	+H	806.4199	806.4204	0.0005	806.4191	-0.0008	-1	18820
	3	-SH	795.0906	795.0921	0.0015	795.0908	0.0002	0	12950
	3	+SH	817.0773	817.0788	0.0015	817.0775	0.0002	0	11410
b23	2	-H	1318.1605	1318.1619	0.0014	1318.1602	-0.0003	0	22660

**Tab. S2 Cont.**

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
b23	2		1318.6645	1318.6621	-0.0024	1318.6604	-0.0041	-3	8860
	2	+H	1319.1684	1319.1654	-0.0030	1319.1637	-0.0048	-4	7540
	3		879.4456	879.4450	-0.0006	879.4437	-0.0020	-2	4650
	3	+H	879.7816	879.7799	-0.0017	879.7786	-0.0030	-3	3040
b26	2	-H	1446.7295	1446.7306	0.0011	1446.7287	-0.0008	-1	1920
	2		1447.2335	1447.2344	0.0009	1447.2325	-0.0009	-1	2430
	2	+H	1447.7374	1447.7379	0.0005	1447.7360	-0.0014	-1	6130
b29	3		1098.2216	1098.2218	0.0002	1098.2203	-0.0014	-1	1350
	3	+H	1098.5576	1098.5585	0.0009	1098.5570	-0.0006	-1	16570
	3	-SH	1087.2283	1087.2314	0.0031	1087.2299	0.0016	1	8850
	3	+SH	1109.2150	1109.2186	0.0036	1109.2171	0.0021	2	22350
b30	3		1132.2223	1132.2242	0.0019	1132.2226	0.0003	0	46880
	3	+H	1132.5583	1132.5581	-0.0002	1132.5565	-0.0017	-2	40340
	3	-SH	1121.2290	1121.2288	-0.0002	1121.2272	-0.0017	-2	15000
	3	+SH	1143.2156	1143.2156	0.0000	1143.2140	-0.0016	-1	5680
b31	3		1155.9013	1155.9031	0.0018	1155.9015	0.0002	0	1360
	3	+H	1156.2373	1156.2386	0.0013	1156.2370	-0.0003	0	15380
	3	+SH	1166.5587	1166.5636	0.0049	1166.5620	0.0033	3	15170
b32	3		1179.5803	1179.5831	0.0028	1179.5815	0.0012	1	1490
	3	+H	1179.9163	1179.9167	0.0004	1179.9151	-0.0012	-1	20950
b33	3		1222.2786	1222.2806	0.0020	1222.2789	0.0003	0	30040
	3	+H	1222.6146	1222.6147	0.0001	1222.6130	-0.0016	-1	26980
b34	3	+H	1271.6373	1271.6377	0.0004	1271.6360	-0.0013	-1	6710
b35	3		1314.3156	1314.3158	0.0002	1314.3141	-0.0016	-1	56830
	3	+H	1314.6516	1314.6514	-0.0002	1314.6497	-0.0019	-1	0
b36	3		1343.3263	1343.3273	0.0010	1343.3255	-0.0008	-1	8780
b37	3		1381.3406	1381.3435	0.0029	1381.3417	0.0011	1	20270
b39	3		1468.3776	1468.3761	-0.0015	1468.3742	-0.0034	-2	30420
b40	3		1502.0603	1502.0668	0.0065	1502.0649	0.0046	3	3300
b44	3		1640.1223	1640.1250	0.0027	1640.1230	0.0007	0	44910
b45	3		1692.1560	1692.1616	0.0056	1692.1595	0.0036	2	92520
	4		1269.3690	1269.3696	0.0006	1269.3679	-0.0010	-1	31250
b46	4		1298.1317	1298.1323	0.0006	1298.1306	-0.0011	-1	25800
b47	4		1323.3937	1323.3940	0.0003	1323.3923	-0.0014	-1	12120
b48	4		1351.8985	1351.9003	0.0018	1351.8985	0.0001	0	423700
	4	+SH	1360.1435	1360.1444	0.0009	1360.1426	-0.0008	-1	68630
	4	-2SH	1335.4084	1335.4061	-0.0023	1335.4043	-0.0041	-3	20890
b49	4		1366.1537	1366.1577	0.0040	1366.1559	0.0022	2	17200
b52	4		1441.9305	1441.9324	0.0019	1441.9305	0.0001	0	144240

Tab. S2 Cont.

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
b59	4	+H	1642.5419	1642.5436	0.0017	1642.5416	-0.0004	0	32785
b63	5		1437.0920	1437.0958	0.0038	1437.0940	0.0020	1	86970
b65	5		1480.3008	1480.3004	-0.0004	1480.2985	-0.0022	-2	42260
	5	-SH	1473.7047	1473.7072	0.0025	1473.7053	0.0006	0	31540
b66	5		1503.3062	1503.3052	-0.0010	1503.3033	-0.0029	-2	46460
	5	-SH	1496.9117	1496.9113	-0.0004	1496.9094	-0.0023	-2	44570
y2	1		288.2030	288.2035	0.0005	288.2027	-0.0003	-1	90300
y3	1	-H	389.1961	389.1972	0.0011	389.1963	0.0002	1	8710
	1	+H	391.2119	391.2128	0.0009	391.2119	0.0000	0	5920
	1	-SH	357.2240	357.2251	0.0011	357.2242	0.0002	1	23590
y4	1	-H	446.2181	446.2189	0.0008	446.2180	-0.0001	0	6950
	1	+H	448.2339	448.2345	0.0006	448.2336	-0.0004	-1	13200
	1	-SH	414.2460	414.2467	0.0007	414.2458	-0.0002	0	17500
	1	+SH	480.2060	480.2066	0.0006	480.2056	-0.0004	-1	5980
y5	1	-H	602.3191	602.3210	0.0019	602.3199	0.0009	1	1930
	1	+H	604.3349	604.3361	0.0012	604.3350	0.0001	0	3510
	1	-SH	570.3470	570.3481	0.0011	570.3470	0.0001	0	2010
y6	1	-H	715.4031	715.4044	0.0013	715.4032	0.0002	0	2060
	1	+H	717.4189	717.4207	0.0018	717.4195	0.0006	1	2480
	1	-SH	683.4310	683.4327	0.0017	683.4315	0.0006	1	2770
y7	1	-H	901.4821	901.4836	0.0015	901.4822	0.0002	0	3270
	1		902.4900	902.4875	-0.0025	902.4861	-0.0039	-4	1370
	1	+H	903.4979	903.5001	0.0022	903.4987	0.0008	1	3210
	1	-SH	869.5100	869.5121	0.0021	869.5108	0.0008	1	6940
y8	1	-H	972.5191	972.5211	0.0020	972.5197	0.0006	1	3870
	1		973.5270	973.5242	-0.0028	973.5228	-0.0042	-4	1640
	1	+H	974.5349	974.5366	0.0017	974.5352	0.0002	0	5160
	1	-SH	940.5470	940.5498	0.0028	940.5484	0.0014	2	7470
y9	1	-H	1100.5781	1100.5858	0.0077	1100.5843	0.0062	6	4020
	1		1101.5860	1101.5825	-0.0035	1101.5810	-0.0050	-5	1760
	1	+H	1102.5939	1102.5968	0.0029	1102.5953	0.0013	1	4810
	1	-SH	973.5270	973.5242	-0.0028	973.5228	-0.0042	-4	2920
y10	1	-H	1199.6461	1199.6489	0.0028	1199.6473	0.0012	1	42000
	1		1200.6540	1200.6521	-0.0019	1200.6505	-0.0035	-3	28700
	1	+H	1201.6619	1201.6652	0.0033	1201.6636	0.0016	1	187040
	1	-SH	1167.6740	1167.6768	0.0028	1167.6752	0.0012	1	204950
	1	+SH	1233.6340	1233.6373	0.0033	1233.6356	0.0016	1	68270
	2	-H	600.3270	600.3281	0.0011	600.3270	0.0000	0	21700
	2		600.8310	600.8301	-0.0009	600.8290	-0.0020	-3	11900

Tab. S2 Cont.

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
y10	2	+H	601.3349	601.3364	0.0015	601.3353	0.0004	1	47720
	2	-SH	584.3410	584.3421	0.0011	584.3410	0.0001	0	76990
	2	+SH	617.3210	617.3221	0.0011	617.3210	0.0000	0	28450
y11	1	-H	1314.6731	1314.6753	0.0022	1314.6736	0.0005	0	5850
	1		1315.6810	1315.6780	-0.0030	1315.6763	-0.0047	-4	4110
	1	+H	1316.6889	1316.6918	0.0029	1316.6901	0.0011	1	51700
	1	-SH	1282.7010	1282.7039	0.0029	1282.7022	0.0012	1	22150
	2	-H	657.8405	657.8417	0.0012	657.8406	0.0001	0	1510
	2		658.3445	658.3460	0.0015	658.3449	0.0004	1	1390
	2	+H	658.8484	658.8495	0.0011	658.8484	-0.0001	0	31090
	2	-SH	641.8545	641.8559	0.0014	641.8548	0.0003	0	6520
	2	-H	736.8755	736.8767	0.0012	736.8755	0.0000	0	1320
y13	2		737.3795	737.3774	-0.0021	737.3762	-0.0033	-4	1030
	2	+H	737.8834	737.8847	0.0013	737.8835	0.0000	0	3780
	2	-SH	720.8895	720.8908	0.0013	720.8896	0.0001	0	4940
	2	+SH	753.8695	753.8700	0.0005	753.8688	-0.0007	-1	1190
	2	-H	800.9225	800.9245	0.0020	800.9232	0.0007	1	4550
y14	2		801.4265	801.4255	-0.0010	801.4242	-0.0022	-3	2830
	2	+H	801.9304	801.9322	0.0018	801.9309	0.0005	1	22940
	2	-SH	784.9365	784.9379	0.0014	784.9366	0.0002	0	20430
	2	+SH	817.4125	817.4132	0.0007	817.4119	-0.0006	-1	20020
	2	-H	851.9235	851.9233	-0.0002	851.9220	-0.0015	-2	1130
y15	2		852.4275	852.4285	0.0010	852.4272	-0.0003	0	19100
	2	+H	852.9314	852.9308	-0.0006	852.9295	-0.0020	-2	23670
	2	-SH	835.9375	835.9368	-0.0007	835.9355	-0.0020	-2	23850
	2	+SH	868.9175	868.9161	-0.0014	868.9148	-0.0027	-3	8040
	2	-2SH	819.4475	819.4489	0.0014	819.4476	0.0002	0	9819
	2		930.4780	930.4798	0.0018	930.4784	0.0004	0	34900
y16	2	+H	930.9819	930.9813	-0.0006	930.9799	-0.0020	-2	21500
	2	-SH	913.4840	913.4859	0.0019	913.4845	0.0005	1	21000
	2	+SH	946.4640	946.4649	0.0009	946.4635	-0.0005	-1	6040
	2	-2SH	897.4980	897.4986	0.0006	897.4972	-0.0007	-1	4620
	2		987.4995	987.5005	0.0010	987.4991	-0.0004	0	11630
y17	2	+H	988.0034	988.0028	-0.0006	988.0014	-0.0021	-2	7240
	2	-SH	971.0095	971.0090	-0.0005	971.0076	-0.0019	-2	7570
	2		1065.5500	1065.5519	0.0019	1065.5504	0.0004	0	3170
y18	2	+H	1066.0539	1066.0535	-0.0004	1066.0520	-0.0019	-2	1820
	2		1243.6425	1243.6422	-0.0003	1243.6405	-0.0019	-2	6710
y21	2		1336.6820	1336.6843	0.0023	1336.6825	0.0006	0	3900

Tab. S2 Cont.

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
y22	3	+H	891.7933	891.7930	-0.0003	891.7916	-0.0016	-2	3090
y24	3	+H	953.4866	953.4865	-0.0001	953.4851	-0.0015	-2	5200
y25	2	-H	1494.2385	1494.2365	-0.0020	1494.2346	-0.0039	-3	1390
	2		1494.7425	1494.7412	-0.0013	1494.7393	-0.0032	-2	1870
	2	+H	1495.2464	1495.2455	-0.0009	1495.2436	-0.0028	-2	13880
y26	2	-H	1522.7490	1522.7485	-0.0005	1522.7466	-0.0024	-2	4050
	2		1523.2530	1523.2560	0.0030	1523.2541	0.0011	1	185690
	2	-SH	1506.7630	1506.7626	-0.0004	1506.7607	-0.0023	-2	102820
	2	+SH	1539.2390	1539.2404	0.0014	1539.2385	-0.0005	0	47080
	2	-2SH	1490.2730	1490.2760	0.0030	1490.2741	0.0011	1	26790
	3		1015.8380	1015.8391	0.0011	1015.8376	-0.0003	0	81990
	3	-SH	1004.8446	1004.8453	0.0007	1004.8438	-0.0008	-1	45640
	3	+SH	1026.4953	1026.4983	0.0030	1026.4968	0.0015	1	17250
	3	-2SH	993.8513	993.8534	0.0021	993.8520	0.0007	1	23010
y27	2	-H	1579.7705	1579.7684	-0.0021	1579.7664	-0.0041	-3	24210
y28	2	-H	1608.2815	1608.2839	0.0024	1608.2819	0.0004	0	4860
	2		1608.7855	1608.7881	0.0026	1608.7861	0.0006	0	50900
	2	+H	1609.2894	1609.2888	-0.0006	1609.2868	-0.0026	-2	279440
	2	-SH	1591.7915	1591.7974	0.0059	1591.7954	0.0039	2	196160
	2	+SH	1624.7715	1624.7716	0.0001	1624.7696	-0.0019	-1	70860
	2	-2SH	1575.3015	1575.2993	-0.0022	1575.2973	-0.0042	-3	45660
	3	-H	1072.5236	1072.5227	-0.0009	1072.5212	-0.0025	-2	3530
	3		1072.8596	1072.8610	0.0014	1072.8595	-0.0001	0	23700
	3	+H	1073.1956	1073.1952	-0.0004	1073.1937	-0.0019	-2	133890
	3	-SH	1061.5303	1061.5320	0.0017	1061.5305	0.0002	0	94720
	3	+SH	1083.5170	1083.5189	0.0019	1083.5174	0.0004	0	32170
	3	-2SH	1050.5370	1050.5375	0.0005	1050.5360	-0.0010	-1	26440
	4		804.8967	804.8969	0.0002	804.8956	-0.0011	-1	4960
	4	+H	805.1487	805.1472	-0.0015	805.1459	-0.0028	-3	3930
y29	2	-H	1665.7945	1665.7952	0.0007	1665.7931	-0.0014	-1	2460
	2		1666.2985	1666.3008	0.0023	1666.2987	0.0003	0	2740
	2	+H	1666.8024	1666.7999	-0.0025	1666.7978	-0.0046	-3	23930
	3		1111.2016	1111.2039	0.0023	1111.2023	0.0007	1	8840
y30	3		1140.2123	1140.2122	-0.0001	1140.2106	-0.0017	-1	12880
y31	3		1173.2353	1173.2356	0.0003	1173.2340	-0.0013	-1	1520
	3	+H	1173.5713	1173.5706	-0.0007	1173.5690	-0.0023	-2	16394
y32	3		1210.9300	1210.9319	0.0019	1210.9303	0.0003	0	18110
y33	3		1253.6283	1253.6299	0.0016	1253.6282	-0.0001	0	17930
y35	3	+H	1320.3416	1320.3409	-0.0007	1320.3392	-0.0024	-2	21970

Tab. S2 Cont.

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
c2	1		245.1970	245.1976	0.0006	245.1968	-0.0002	-1	51330
c3	1		392.2660	392.2663	0.0003	392.2654	-0.0006	-2	185000
c4	1		449.2870	449.2879	0.0009	449.2870	0.0000	0	141140
c5	1		605.3880	605.3895	0.0015	605.3884	0.0004	1	504950
c6	1	-H	706.3821	706.3833	0.0012	706.3821	0.0001	0	2010
	1	+H	708.3979	708.3991	0.0012	708.3979	0.0000	0	22060
	1	-SH	674.4100	674.4111	0.0011	674.4099	0.0000	0	10720
	1	+SH	740.3700	740.3709	0.0009	740.3697	-0.0003	0	2860
c7	1	-H	835.4241	835.4258	0.0017	835.4245	0.0004	1	4110
	1		836.4320	836.4317	-0.0003	836.4304	-0.0016	-2	1810
	1	+H	837.4399	837.4418	0.0019	837.4405	0.0006	1	31350
	1	-SH	803.4520	803.4540	0.0020	803.4527	0.0007	1	11930
	1	+SH	869.4120	869.4139	0.0019	869.4126	0.0006	1	6990
c8	1	-H	948.5081	948.5109	0.0028	948.5095	0.0014	2	3970
	1		949.5160	949.5185	0.0025	949.5171	0.0011	1	5090
	1	+H	950.5239	950.5260	0.0021	950.5246	0.0007	1	33650
	1	-SH	916.5360	916.5385	0.0025	916.5371	0.0011	1	9260
	1	+SH	982.4960	982.4980	0.0020	982.4966	0.0006	1	17450
c9	1	-H	1019.5451	1019.5474	0.0023	1019.5459	0.0009	1	7110
	1		1020.5530	1020.5551	0.0021	1020.5536	0.0006	1	9590
	1	+H	1021.5609	1021.5634	0.0025	1021.5619	0.0010	1	52760
	1	-SH	987.5730	987.5756	0.0026	987.5742	0.0012	1	15590
	1	+SH	1053.5330	1053.5345	0.0015	1053.5330	0.0000	0	13030
c10	1	-H	1090.5821	1090.5850	0.0029	1090.5835	0.0014	1	7680
	1		1091.5900	1091.5911	0.0011	1091.5896	-0.0004	0	9310
	1	+H	1092.5979	1092.6003	0.0024	1092.5988	0.0008	1	47760
	1	-SH	1058.6100	1058.6123	0.0023	1058.6108	0.0008	1	17640
	1	+SH	1123.5621	1123.5640	0.0019	1123.5624	0.0004	0	14480
c11	1	-H	1161.6201	1161.6219	0.0018	1161.6203	0.0002	0	2550
	1		1162.6280	1162.6283	0.0003	1162.6267	-0.0013	-1	3690
	1	+H	1163.6359	1163.6372	0.0013	1163.6356	-0.0003	0	26780
	1	-SH	1129.6480	1129.6495	0.0015	1129.6479	-0.0001	0	10520
	1	+SH	1195.6080	1195.6086	0.0006	1195.6070	-0.0010	-1	7750
c12	1	-H	1292.6601	1292.6622	0.0021	1292.6605	0.0004	0	5770
	1		1293.6680	1293.6711	0.0031	1293.6694	0.0014	1	20000
	1	+H	1294.6759	1294.6781	0.0022	1294.6764	0.0004	0	137400
	1	-SH	1260.6880	1260.6903	0.0023	1260.6886	0.0006	0	39670
	1	+SH	1326.6480	1326.6498	0.0018	1326.6481	0.0000	0	24460
c13	1	-H	1420.7551	1420.7584	0.0033	1420.7566	0.0015	1	3360

Tab. S2 Cont.

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
c13	1		1421.7630	1421.7635	0.0005	1421.7617	-0.0013	-1	5580
	1	+H	1422.7709	1422.7734	0.0025	1422.7716	0.0006	0	33840
	1	-SH	1388.7830	1388.7855	0.0025	1388.7837	0.0007	1	14250
	1	+SH	1454.7430	1454.7443	0.0013	1454.7424	-0.0006	0	6600
	2	+H	711.8894	711.8915	0.0021	711.8903	0.0009	1	1130
c14	1	-H	1576.8561	1576.8606	0.0045	1576.8586	0.0026	2	1340
	1		1577.8640	1577.8660	0.0020	1577.8640	0.0000	0	3320
	1	+H	1578.8719	1578.8733	0.0014	1578.8713	-0.0006	0	16830
	1	-SH	1544.8840	1544.8872	0.0032	1544.8853	0.0013	1	4850
	1	+SH	1610.8440	1610.8505	0.0065	1610.8485	0.0045	3	1530
	2	-H	788.9320	788.9334	0.0014	788.9321	0.0001	0	2350
	2		789.4360	789.4362	0.0002	789.4349	-0.0010	-1	3200
	2	+H	789.9399	789.9413	0.0014	789.9400	0.0001	0	17780
	2	-SH	772.9460	772.9476	0.0016	772.9464	0.0004	1	8880
	2	+SH	805.9260	805.9268	0.0008	805.9255	-0.0004	-1	3960
c15	2	-H	857.4615	857.4629	0.0014	857.4616	0.0001	0	10400
	2		857.9655	857.9655	0.0000	857.9642	-0.0013	-2	9860
	2	+H	858.4694	858.4710	0.0016	858.4697	0.0002	0	38390
	2	-SH	841.4755	841.4768	0.0013	841.4755	0.0000	0	15400
	2	+SH	874.4555	874.4554	-0.0001	874.4541	-0.0014	-2	9420
c16	2	-H	885.9720	885.9735	0.0015	885.9722	0.0002	0	3440
	2		886.4760	886.4736	-0.0024	886.4723	-0.0037	-4	33200
	2	+H	886.9799	886.9815	0.0016	886.9802	0.0002	0	27430
	2	-SH	869.9860	869.9878	0.0018	869.9865	0.0005	1	13240
	2	+SH	902.9660	902.9676	0.0016	902.9662	0.0003	0	7580
c17	2	-H	942.5145	942.5156	0.0011	942.5142	-0.0003	0	6750
	2		943.0185	943.0182	-0.0003	943.0168	-0.0017	-2	9710
	2	+H	943.5224	943.5240	0.0016	943.5226	0.0002	0	59500
	2	-SH	926.5285	926.5300	0.0015	926.5286	0.0002	0	37590
	2	+SH	959.5085	959.5083	-0.0002	959.5069	-0.0016	-2	27370
c18	2	-H	1000.0275	1000.0294	0.0019	1000.0280	0.0005	0	6380
	2		1000.5315	1000.5316	0.0001	1000.5302	-0.0013	-1	9390
	2	+H	1001.0354	1001.0372	0.0018	1001.0357	0.0003	0	71300
	2	-SH	984.0415	984.0433	0.0018	984.0419	0.0004	0	44050
	2	+SH	1017.0215	1017.0234	0.0019	1017.0219	0.0005	0	23230
c19	2	-H	1057.0490	1057.0520	0.0030	1057.0505	0.0015	1	2130
	2		1057.5530	1057.5546	0.0016	1057.5531	0.0001	0	1220
	2	+H	1058.0569	1058.0608	0.0039	1058.0593	0.0024	2	28370
	2	-SH	1041.0630	1041.0657	0.0027	1041.0642	0.0012	1	21690

Tab. S2 Cont.

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
c19	2	+SH	1074.0430	1074.0444	0.0014	1074.0429	-0.0001	0	5740
c20	2	-H	1138.5810	1138.5830	0.0020	1138.5814	0.0004	0	4620
	2		1139.0850	1139.0850	0.0000	1139.0834	-0.0015	-1	8110
	2	+H	1139.5889	1139.5903	0.0014	1139.5887	-0.0002	0	63300
	2	-SH	1122.5950	1122.5968	0.0018	1122.5952	0.0003	0	31170
	2	+SH	1155.0710	1155.0715	0.0005	1155.0699	-0.0011	-1	20370
c21	2	-H	1216.6315	1216.6317	0.0002	1216.6301	-0.0014	-1	5200
	2		1217.1355	1217.1357	0.0002	1217.1341	-0.0014	-1	6580
	2	+H	1217.6394	1217.6398	0.0004	1217.6382	-0.0013	-1	51100
	2	+SH	1234.1294	1234.1281	-0.0013	1234.1264	-0.0030	-2	9800
	3		811.7596	811.7587	-0.0009	811.7574	-0.0022	-3	1070
c22	3	+H	812.0956	812.0963	0.0007	812.0950	-0.0006	-1	3310
	2	-H	1245.1420	1245.1458	0.0038	1245.1441	0.0021	2	2390
	2		1245.6460	1245.6462	0.0002	1245.6445	-0.0014	-1	3350
	2	+H	1246.1499	1246.1505	0.0006	1246.1488	-0.0011	-1	27250
	2	-SH	1229.1560	1229.1581	0.0021	1229.1564	0.0005	0	9940
c23	2	+SH	1262.1360	1262.1343	-0.0017	1262.1326	-0.0034	-3	14560
	3	-H	830.4306	830.4319	0.0013	830.4306	0.0000	0	705
	3	+H	831.1026	831.1029	0.0003	831.1016	-0.0010	-1	2730
	2	-H	1326.6740	1326.6770	0.0030	1326.6753	0.0013	1	6840
	2		1327.1780	1327.1781	0.0001	1327.1764	-0.0016	-1	9810
	2	+H	1327.6819	1327.6829	0.0010	1327.6812	-0.0008	-1	78400
	2	-SH	1310.6880	1310.6896	0.0016	1310.6879	-0.0001	0	23970
c24	3		885.1213	885.1228	0.0015	885.1215	0.0002	0	2180
	3	+H	885.4573	885.4579	0.0006	885.4566	-0.0007	-1	14660
	3	+SH	896.1146	896.1147	0.0001	896.1133	-0.0013	-1	2800
	2	-H	1370.1900	1370.1921	0.0021	1370.1903	0.0003	0	2110
	2		1370.6940	1370.6926	-0.0014	1370.6908	-0.0032	-2	3830
	2	+H	1371.1979	1371.1978	-0.0001	1371.1960	-0.0019	-1	29790
	2	-SH	1354.2040	1354.2064	0.0024	1354.2046	0.0007	0	20720
c25	2	+SH	1387.1840	1387.1840	0.0000	1387.1822	-0.0018	-1	7185
	3	+H	914.4679	914.4684	0.0005	914.4670	-0.0009	-1	7940
	2	+H	1427.7399	1427.7406	0.0007	1427.7388	-0.0012	-1	15320
	3	+H	971.1696	971.1698	0.0002	971.1684	-0.0012	-1	8400
	2	-H	1455.2425	1455.2454	0.0029	1455.2435	0.0010	1	1180
c26	2		1455.7465	1455.7480	0.0015	1455.7461	-0.0003	0	6290
	2	+H	1456.2504	1456.2518	0.0014	1456.2499	-0.0005	0	31120
	2	-SH	1439.2565	1439.2584	0.0019	1439.2566	0.0001	0	25020
c27	2	+H	1513.2719	1513.2728	0.0009	1513.2709	-0.0011	-1	9550



Tab. S2 Cont.

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
c27	3	+H	1009.1839	1009.1852	0.0013	1009.1837	-0.0002	0	1160
c29	3	+H	1104.2333	1104.2329	-0.0004	1104.2314	-0.0019	-2	21310
	3	-SH	1092.9040	1092.9063	0.0023	1092.9048	0.0008	1	10140
	3	+SH	1114.8906	1114.8922	0.0016	1114.8906	0.0000	0	21390
c34	3		1276.9770	1276.9790	0.0020	1276.9773	0.0003	0	3170
c36	3		1349.0016	1349.0031	0.0015	1349.0013	-0.0003	0	37170
	3	+H	1349.3376	1349.3381	0.0005	1349.3363	-0.0013	-1	30380
c37	3		1387.0160	1387.0156	-0.0004	1387.0138	-0.0022	-2	10528.5
	3	+H	1387.3519	1387.3523	0.0004	1387.3505	-0.0014	-1	8820
c39	3	+H	1474.3893	1474.3925	0.0032	1474.3906	0.0013	1	11200
c40	3		1507.7356	1507.7397	0.0041	1507.7378	0.0022	1	21640
c41	3	+H	1551.0939	1551.0912	-0.0027	1551.0892	-0.0047	-3	6690
c42	3	+H	1574.4369	1574.4373	0.0004	1574.4353	-0.0016	-1	9015
c43	3		1607.7836	1607.7865	0.0029	1607.7845	0.0009	1	41900
c44	3		1645.7980	1645.8051	0.0071	1645.8031	0.0051	3	7430
c45	3		1697.8316	1697.8345	0.0029	1697.8324	0.0008	0	113800
	4		1273.6257	1273.6309	0.0052	1273.6292	0.0035	3	19510
c46	4		1302.1365	1302.1385	0.0020	1302.1368	0.0003	0	14320
	4	+H	1302.3884	1302.3878	-0.0006	1302.3861	-0.0024	-2	12900
c49	4	+H	1370.6624	1370.6641	0.0017	1370.6623	-0.0001	0	9670
c50	4	+H	1392.6724	1392.6721	-0.0003	1392.6703	-0.0021	-2	5980
c51	4	+H	1417.6824	1417.6848	0.0024	1417.6830	0.0005	0	11150
c53	4	+H	1487.2049	1487.2072	0.0023	1487.2053	0.0004	0	9085
c58	4	+H	1618.5399	1618.5363	-0.0036	1618.5343	-0.0056	-3	4470
c63	5		1440.4974	1440.4993	0.0019	1440.4974	0.0001	0	53120
	5	+SH	1447.2949	1447.2933	-0.0016	1447.2914	-0.0035	-2	3940
c64	5	+H	1461.0991	1461.0995	0.0004	1461.0976	-0.0015	-1	9430
c65	5	+H	1484.1093	1484.1062	-0.0031	1484.1043	-0.0050	-3	5630
z2	1		271.1760	271.1769	0.0009	271.1761	0.0001	0	12110
z3	1		373.1780	373.1784	0.0004	373.1775	-0.0005	-1	7640
	1	+H	374.1859	374.1862	0.0003	374.1853	-0.0006	-2	14800
	1	-SH	340.1980	340.1985	0.0005	340.1977	-0.0003	-1	9040
z4	1	-H	429.1911	429.1924	0.0013	429.1915	0.0004	1	1550
	1		430.1990	430.2000	0.0010	430.1991	0.0001	0	1530
	1	+H	431.2069	431.2079	0.0010	431.2070	0.0000	0	12800
	1	-SH	397.2190	397.2198	0.0008	397.2189	-0.0001	0	1100
z5	1	-H	585.2921	585.2938	0.0017	585.2927	0.0007	1	2960
	1	+H	587.3079	587.3092	0.0013	587.3081	0.0002	0	5570
	1	-SH	553.3200	553.3223	0.0023	553.3213	0.0013	2	1160

Tab. S2 Cont.

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
z6	1	-H	698.3761	698.3784	0.0023	698.3772	0.0012	2	1600
	1	+H	700.3919	700.3939	0.0020	700.3927	0.0008	1	23000
	1	-SH	666.4040	666.4065	0.0025	666.4054	0.0014	2	1310
z7	1	-H	884.4561	884.4565	0.0004	884.4552	-0.0009	-1	4680
	1	+H	886.4719	886.4736	0.0017	886.4723	0.0003	0	33200
	1	-SH	852.4840	852.4857	0.0017	852.4844	0.0004	0	8320
z8	1	+SH	918.4440	918.4445	0.0005	918.4431	-0.0009	-1	2540
	1	-H	955.4931	955.4943	0.0012	955.4929	-0.0002	0	3120
	1	+H	957.5089	957.5107	0.0018	957.5093	0.0003	0	36400
z9	1	-SH	923.5210	923.5234	0.0024	923.5220	0.0010	1	4210
	1	+SH	989.4810	989.4830	0.0020	989.4816	0.0005	1	2540
	1	-H	1083.5511	1083.5524	0.0013	1083.5509	-0.0002	0	2750
z10	1		1084.5590	1084.5563	-0.0027	1084.5548	-0.0042	-4	1300
	1	+H	1085.5669	1085.5695	0.0026	1085.5680	0.0010	1	31500
	1	-SH	1051.5790	1051.5815	0.0025	1051.5800	0.0010	1	3370
	1	+SH	1117.5390	1117.5417	0.0027	1117.5401	0.0011	1	1620
	1	-H	1182.6201	1182.6227	0.0026	1182.6211	0.0010	1	16700
z11	1		1183.6280	1183.6261	-0.0019	1183.6245	-0.0035	-3	10800
	1	+H	1184.6359	1184.6392	0.0033	1184.6376	0.0016	1	12500
	1	-SH	1150.6480	1150.6503	0.0023	1150.6487	0.0007	1	32450
	1	+SH	1216.6080	1216.6115	0.0035	1216.6099	0.0018	2	5640
	1	-H	1297.6471	1297.6484	0.0013	1297.6467	-0.0004	0	7190
z12	1		1298.6550	1298.6555	0.0005	1298.6538	-0.0012	-1	4470
	1	+H	1299.6629	1299.6678	0.0049	1299.6661	0.0031	2	19100
	1	-SH	1265.6750	1265.6772	0.0022	1265.6755	0.0005	0	31300
	1	+SH	1331.6350	1331.6346	-0.0004	1331.6328	-0.0022	-2	6470
	1	-H	1398.6951	1398.6986	0.0035	1398.6968	0.0017	1	5180
z14	1		1399.7030	1399.7028	-0.0002	1399.7010	-0.0020	-1	4740
	1	+H	1400.7109	1400.7124	0.0015	1400.7106	-0.0004	0	50500
	1	-SH	1366.7230	1366.7214	-0.0016	1366.7196	-0.0034	-2	12085
	1	+SH	1432.6830	1432.6838	0.0008	1432.6820	-0.0011	-1	2350
	2	+H	700.8594	700.8604	0.0010	700.8592	-0.0002	0	7440
z14	1	-H	1583.8111	1583.8164	0.0053	1583.8144	0.0034	2	55200
	1		1584.8190	1584.8137	-0.0053	1584.8117	-0.0073	-5	20900
	1	+H	1585.8269	1585.8229	-0.0040	1585.8209	-0.0060	-4	7000
	2	-H	792.4095	792.4121	0.0026	792.4108	0.0013	2	8080
	2		792.9135	792.9125	-0.0010	792.9112	-0.0022	-3	7670
	2	+H	793.4174	793.4175	0.0001	793.4162	-0.0012	-2	3090
	2	+SH	809.4035	809.4035	0.0000	809.4022	-0.0013	-2	4200

Tab. S2 Cont.

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
z15	1	-H	1685.8121	1685.8109	-0.0012	1685.8088	-0.0032	-2	7090
	1		1686.8200	1686.8224	0.0024	1686.8203	0.0003	0	39700
	1	+H	1687.8279	1687.8257	-0.0022	1687.8236	-0.0043	-3	28200
	1	-SH	1653.8400	1653.8398	-0.0002	1653.8378	-0.0022	-1	106900
	2		843.9140	843.9152	0.0012	843.9139	-0.0001	0	3460
	2	+H	844.4179	844.4179	0.0000	844.4166	-0.0013	-2	5530
	2	-SH	827.4240	827.4241	0.0001	827.4228	-0.0012	-1	13950
z16	2		921.9645	921.9661	0.0016	921.9647	0.0003	0	3360
	2	+H	922.4684	922.4692	0.0008	922.4678	-0.0006	-1	7240
z17	2		978.9860	978.9877	0.0017	978.9863	0.0003	0	8880
	2	+H	979.4899	979.4896	-0.0003	979.4882	-0.0018	-2	9440
	2	-SH	962.4960	962.4944	-0.0016	962.4930	-0.0030	-3	11950
	2	+SH	994.9720	994.9730	0.0010	994.9716	-0.0005	0	3690
z18	2		1057.0365	1057.0381	0.0016	1057.0366	0.0001	0	2210
	2	+H	1057.5404	1057.5420	0.0016	1057.5405	0.0001	0	6100
	2	-SH	1040.5465	1040.5450	-0.0015	1040.5435	-0.0030	-3	5350
z19	2		1150.0765	1150.0784	0.0019	1150.0768	0.0003	0	7610
	2	+H	1150.5804	1150.5796	-0.0008	1150.5780	-0.0024	-2	8770
	2	-SH	1134.0904	1134.0916	0.0012	1134.0900	-0.0004	0	7600
	3		767.0536	767.0544	0.0008	767.0532	-0.0005	-1	1840
	3	+H	767.3896	767.3883	-0.0013	767.3871	-0.0025	-3	1890
	3	-SH	756.7322	756.7316	-0.0006	756.7304	-0.0019	-2	1130
z20	2		1185.5950	1185.5953	0.0003	1185.5937	-0.0013	-1	5470
	2	+H	1186.0989	1186.0975	-0.0014	1186.0959	-0.0031	-3	3960
	2	-SH	1169.6089	1169.6117	0.0028	1169.6101	0.0012	1	4930
z21	2		1235.1290	1235.1302	0.0012	1235.1285	-0.0004	0	5360
	2	+H	1235.6329	1235.6327	-0.0002	1235.6310	-0.0019	-2	6670
	2	+SH	1251.6190	1251.6221	0.0031	1251.6204	0.0014	1	1170
z22	2	+H	1329.1769	1329.1786	0.0017	1329.1769	-0.0001	0	0
	3	+H	886.1179	886.1174	-0.0005	886.1161	-0.0019	-2	2610
z23	2	+H	1364.1914	1364.1929	0.0015	1364.1911	-0.0003	0	4870
	3	+H	909.7969	909.7972	0.0003	909.7958	-0.0011	-1	1280
z24	2		1420.7090	1420.7122	0.0032	1420.7104	0.0014	1	5950
	2	+H	1421.2129	1421.2135	0.0006	1421.2117	-0.0013	-1	9000
	3		947.4753	947.4750	-0.0003	947.4736	-0.0017	-2	1480
	3	+H	947.8113	947.8115	0.0002	947.8101	-0.0012	-1	2510
	3	-SH	937.1539	937.1561	0.0022	937.1547	0.0008	1	2430
	3	+SH	958.4686	958.4699	0.0013	958.4685	-0.0001	0	2210
z25	3	+H	991.4913	991.4961	0.0048	991.4947	0.0034	3	0

**Tab. S2 Cont.**

ID	charge state	modification	theoretical m/z (Th)	measured m/z (Th)	absolute error (Th)	recalibrated m/z <sup>1</sup> (Th)	recalibrated error (Th)	relative error <sup>2</sup> (ppm)	Intensity <sup>3</sup>
z26	3		1010.1626	1010.1650	0.0024	1010.1635	0.0009	1	3460
	3	+H	1010.4986	1010.4968	-0.0018	1010.4953	-0.0033	-3	4570
	3	-SH	998.8333	998.8369	0.0036	998.8355	0.0021	2	8450
z27	3	+H	1048.8489	1048.8475	-0.0014	1048.8460	-0.0029	-3	0
	3	-SH	1037.5196	1037.5176	-0.0020	1037.5161	-0.0035	-3	5650
z28	3		1067.1840	1067.1857	0.0017	1067.1842	0.0002	0	23060
	3	+SH	1077.8413	1077.8440	0.0027	1077.8425	0.0012	1	4390
z29	3		1105.5263	1105.5275	0.0012	1105.5260	-0.0003	0	1120
	3	+H	1105.8623	1105.8638	0.0015	1105.8623	0.0000	0	1530
z30	3	+H	1134.8729	1134.8737	0.0008	1134.8721	-0.0008	-1	2640
z31	3		1167.5596	1167.5636	0.0040	1167.5620	0.0024	2	7490
z32	3		1205.2543	1205.2596	0.0053	1205.2580	0.0037	3	6990
z33	3		1247.9526	1247.9551	0.0025	1247.9534	0.0008	1	5620
z34	3	+H	1290.9869	1290.9878	0.0009	1290.9861	-0.0009	-1	2020
z36	3	+H	1349.0026	1349.0031	0.0005	1349.0013	-0.0013	-1	0
	3	-SH	1337.3373	1337.3396	0.0023	1337.3378	0.0006	0	24810
z37	3	+H	1386.6809	1386.6818	0.0009	1386.6800	-0.0009	-1	0
z41	3	+H	1506.0759	1506.0781	0.0022	1506.0762	0.0002	0	1970
z42	3		1543.4346	1543.4404	0.0058	1543.4385	0.0038	2	6200
z45	3	+H	1640.1343	1640.1350	0.0007	1640.1330	-0.0013	-1	2000

1. Recalibrated using the equation: recalibrated m/z = (measured m/z) - (measured m/z)\* $k$  -  $b$ , where  $k=9.11485*10^{-7}$ ,  $b=5.37764*10^{-4}$ , (determined by linear fitting of the (absolute error) vs. (measured m/z) data) ;

2. Error tolerance was set as  $\pm 3$  ppm for F $\pm$ SH ions and the smallest F+nH (n=-1, 0, 1) ions, and  $\pm 6$  ppm for F+(n+1)H (n=-1, 0, 1) ions, because the contribution of <sup>13</sup>C;

3. For F $\pm$ H species, additional deconvolution is needed to determine the abundances of F-H, F and F+H (see Results section for detail).