

Meas. m/z	Calc. m/z	Delta (Da)	Delta (ppm)	Rel. Int. (%)	Annotation	Formula
1547.6906	1547.6438	0.0467	30.2	8.24	[b14][1-14].GRASCKKCESEIPK.d [1xArsenicBinding]	AsC60H103N20O19S2
1590.8248	1590.7727	0.0521	32.8	53.29	[b15][1-15].GRASCKKCESEIPK.k	C64H111N21O22S2
1594.49	1594.5706	-0.0806	-50.5	7.22	[y-NH3-11][19-29] p.HWYHFSCFWKV. [1xArsenicBinding]	AsC78H88N17O14S
1636.8436	1636.7518	0.0918	56.1	13.83	[y12][18-29] v.PHWYHFSCFWKV.	C83H101N19O15S
1644.7253	1644.6602	0.0651	39.6	7.11	[b-H2O-15][1-15].GRASCKKCESEIPK.k [1xArsenicBinding]	AsC64H106N21O21S2
1645.7014	1645.6442	0.0572	34.8	10.19	[b-NH3-15][1-15].GRASCKKCESEIPK.k [1xArsenicBinding]	AsC64H105N20O22S2
1662.7295	1662.6708	0.0587	35.3	100	[b15][1-15].GRASCKKCESEIPK.k [1xArsenicBinding]	AsC64H108N21O22S2
1708.634	1708.6499	-0.0159	-9.3	6.16	[y12][18-29] v.PHWYHFSCFWKV. [1xArsenicBinding]	AsC83H98N19O15S
1789.8946	1789.9411	-0.0466	-26	6.12	[a17][1-17].GRASCKKCESEIPKDKV.p	C74H132N24O23S2
1861.8605	1861.8393	0.0212	11.4	6.12	[a17][1-17].GRASCKKCESEIPKDKV.p [1xArsenicBinding]	AsC74H129N24O23S2
1863.9980	1863.9152	0.0828	44.4	17.01	[y14][16-29] d.KVPHWYHFSCFWKV.	C94H122N22O17S
1889.8873	1889.8342	0.0531	28.1	7.81	[b17][1-17].GRASCKKCESEIPKDKV.p [1xArsenicBinding]	AsC75H129N24O24S2
1935.8337	1935.8133	0.0204	10.5	9.51	[y14][16-29] d.KVPHWYHFSCFWKV. [1xArsenicBinding]	AsC94H119N22O17S
2404.21	2404.2059	0.004	1.7	5.56	[y19][11-29] e.SIPKDKVPHWYHFSCFWKV.	C118H162N28O25S
2755.4611	2755.3232	0.1379	50.1	5.23	[b-NH3-24][1-24].GRASCKKCESEIPKDKVPHWYHFS.c	C124H183N35O33S2
3378.6471	3378.6485	-0.0015	-0.4	5.78	[y-H2O-28][2-29] g.RASCKKCESEIPKDKVPHWYHFSCFWKV.	C156H228N42O37S3

Supplemental Table 2. Summary of fragment ions produced by AsPARPzf. The calculated (Calc.) and measured (Meas.) m/z, differences (Delta (Da/ppm)), relative intensity (Rel. Int.), sequences and formulas relating to Figure 2.