Supplementary data

Table 1. Average mass measurement errors of the identified peptides for tryptic digestion of BSA during a multiplexed LC-CID-FTICR-MS separation (before COFI)

		mass tol. = 0.2 Da		mass tol. = 0.1 Da		mass tol. = 0.02 Da	
File #	Sequence	No. of fragment	average absoulte error (ppm)	No. of fragment	average absolute error (ppm)	No. of fragment	average absolute error (ppm)
484	FKDLGEEHFK	11	89.2	4	48.47	0	N/D
486	FKDLGEEHFK	8	95.35	2	59.15	0	N/D
488	FKDLGEEHFK	12	88.29	5	53.77	0	N/D
490	FKDLGEEHFK	10	97.49	3	44.27	0	N/D
492	FKDLGEEHFK	10	96.5	3	43.76	0	N/D
494	FKDLGEEHFK	8	99.99	3	55.68	0	N/D
496	FKDLGEEHFK	6	109.6	2	67.36	0	N/D
498	DAFLGSFLYEYSR	2	102.51	0	N/D	0	N/D
498	FKDLGEEHFK	3	103.76	0	N/D	0	N/D
500	DAFLGSFLYEYSR	2	103.36	0	N/D	0	N/D
506	FKDLGEEHFK	2	108.38	0	N/D	0	N/D
508	FKDLGEEHFK	2	67.12	0	N/D	0	N/D
518	FKDLGEEHFK	3	128.61	0	N/D	0	N/D
528	HLVDEPQNLIK	7	86.18	3	45.11	0	N/D
530	HLVDEPQNLIK	9	90.95	4	48.02	0	N/D
532	HLVDEPQNLIK	9	91.33	4	48.36	0	N/D
534	HLVDEPQNLIK	9	90.76	4	48.12	0	N/D
536	HLVDEPQNLIK	9	90.48	5	47.89	0	N/D
538	HLVDEPQNLIK	8	83.46	4	47.81	0	N/D
538	LVVSTQTALA	2	154.1	0	N/D	0	N/D
538	YLYEIAR	2	115.66	0	N/D	0	N/D
540	HLVDEPQNLIK	8	83.2	4	47.73	0	N/D
540	LVVSTQTALA	3	140.52	0	N/D	0	N/D
540	YLYEIAR	2	115.48	0	N/D	0	N/D
542	HLVDEPQNLIK	6	89.31	2	47.54	0	N/D
542	YLYEIAR	3	97.71	2	78.79	0	N/D
544	HLVDEPQNLIK	7	94.77	3	34.88	1	11.49
544	YLYEIAR	3	95.9	2	77.01	0	N/D
546	HLVDEPQNLIK	5	74.68	2	45.97	0	N/D
546	YLYEIAR	3	93.6	2	76.04	0	N/D

548	HLVDEPQNLIK	4	71.95	2	46.54	0	N/D
548	YLYEIAR	3	95.58	2	77.17	0	N/D
552	HLVDEPQNLIK	4	97.26	1	42.11	0	N/D
552	YLYEIAR	3	96.3	2	31.51	0	N/D
554	YLYEIAR	2	118.25	0	N/D	0	N/D
556	LKHLVDEPQNLIK	3	64.07	0	N/D	0	N/D
558	LKHLVDEPQNLIK	3	64.33	0	N/D	0	N/D
558	YLYEIAR	2	77.6	2	77.43	1	3.82
564	HLVDEPQNLIK	3	84.66	0	N/D	0	N/D
566	YLYEIAR	3	95.33	2	76.5	1	4.4
568	KVPQVSTPTLVEVSR	6	65.97	2	38.61	0	N/D
570	KVPQVSTPTLVEVSR	9	73.83	5	40.04	0	N/D
572	KVPQVSTPTLVEVSR	9	61.39	5	39	0	N/D
574	KVPQVSTPTLVEVSR	7	62.93	3	39.3	0	N/D
576	KVPQVSTPTLVEVSR	7	74.59	3	45.04	0	N/D
578	KVPQVSTPTLVEVSR	10	65.1	5	45.6	0	N/D
580	KVPQVSTPTLVEVSR	8	57.62	3	29.87	0	N/D
582	KVPQVSTPTLVEVSR	9	67.44	4	35.04	0	N/D
584	KVPQVSTPTLVEVSR	7	61.2	5	39.61	0	N/D
586	KVPQVSTPTLVEVSR	6	65.49	2	33.99	0	N/D
588	KVPQVSTPTLVEVSR	6	59.69	4	42.94	0	N/D
590	KVPQVSTPTLVEVSR	7	65.8	3	43.19	0	N/D
592	KVPQVSTPTLVEVSR	4	59.9	2	38.04	0	N/D
594	KVPQVSTPTLVEVSR	5	51.96	3	42.52	0	N/D
596	KVPQVSTPTLVEVSR	4	59.84	2	37.73	0	N/D
598	KVPQVSTPTLVEVSR	3	45.84	2	38.07	0	N/D
602	KVPQVSTPTLVEVSR	3	46.09	2	37.92	0	N/D
632	HLVDEPQNLIK	2	79.38	0	N/D	0	N/D
636	HLVDEPQNLIK	2	80.03	0	N/D	0	N/D
642	HLVDEPQNLIK	2	79.95	1	55.32	0	N/D
644	HLVDEPQNLIK	3	95.85	0	N/D	0	N/D
644	LVNELTEFAK	7	78.35	2	37.15	0	N/D
648	LVNELTEFAK	6	81.67	4	42.99	1	3.65
650	LVNELTEFAK	7	75.06	4	46.79	1	4.34
652	LVNELTEFAK	6	81.1	4	37.63	1	4.34
654	LVNELTEFAK	5	96.78	3	37.93	1	4.6
656	LVNELTEFAK	6	86.24	2	54.85	1	2.79
658	LVNELTEFAK	6	81.21	4	56.86	0	N/D
660	LVNELTEFAK	6	81.56	3	37.93	0	N/D
662	LVNELTEFAK	5	97.21	3	38.21	0	N/D
664	LVNELTEFAK	5	96.73	2	55.32	0	N/D
666	LVNELTEFAK	5	96.67	2	54.98	0	N/D
668	LVNELTEFAK	5	100.29	2	54.72	0	N/D
670	LVNELTEFAK	4	107.71	1	56.33	0	N/D
672	LVNELTEFAK	4	107.95	1	56.01	0	N/D
674	KQTALVELLK	9	98.95	2	65.87	0	N/D
674	LVNELTEFAK	4	111.13	1	63.45	0	N/D
676	KQTALVELLK	10	96.48	3	64.35	0	N/D
676	RHPEYAVSVLLR	3	96.22	1	42.33	0	N/D
678	KQTALVELLK	8	109.52	2	55.24	0	N/D

678	LVNELTEFAK	4	116.03	1	43.01	0	N/D
678	RHPEYAVSVLLR	10	74.88	2	30.13	0	N/D
680	KQTALVELLK	8	104	5	50.94	0	N/D
680	RHPEYAVSVLLR	10	72.83	2	32.13	0	N/D
682	KQTALVELLK	6	96.43	3	43.76	0	N/D
682	RHPEYAVSVLLR	10	82.4	2	57.5	0	N/D
684	KQTALVELLK	6	97.29	3	43.27	0	N/D
684	RHPEYAVSVLLR	8	80.62	2	57.72	0	N/D
686	KQTALVELLK	8	103.59	3	53.61	0	N/D
686	RHPEYAVSVLLR	8	70.58	2	58.56	0	N/D
688	KQTALVELLK	7	93.74	3	43.73	0	N/D
688	RHPEYAVSVLLR	11	82.05	3	63.03	0	N/D
690	KQTALVELLK	2	132.11	0	N/D	0	N/D
690	LVNELTEFAK	3	106.31	0	N/D	0	N/D
690	RHPEYAVSVLLR	9	66.9	4	49.85	0	N/D
692	KQTALVELLK	7	96.62	4	47.47	0	N/D
692	RHPEYAVSVLLR	8	70.34	2	57.72	0	N/D
694	RHPEYAVSVLLR	11	81.22	3	43.55	0	N/D
698	KQTALVELLK	6	101.11	2	50.11	0	N/D
698	RHPEYAVSVLLR	8	69.7	4	57.13	0	N/D
700	RHPEYAVSVLLR	8	85.48	4	49.53	0	N/D
702	LVNELTEFAK	2	128.16	0	N/D	0	N/D
702	RHPEYAVSVLLR	9	58.1	2	44.36	0	N/D
704	KQTALVELLK	8	102.6	6	47.35	0	N/D
704	RHPEYAVSVLLR	9	76.37	2	57.85	0	N/D
706	KQTALVELLK	3	95.85	0	N/D	0	N/D
706	RHPEYAVSVLLR	6	91.22	3	43.57	0	N/D
708	RHPEYAVSVLLR	4	72.48	1	47.56	0	N/D
712	RHPEYAVSVLLR	3	109.88	1	42.34	0	N/D
714	RHPEYAVSVLLR	4	112.96	1	53.12	0	N/D
716	HPEYAVSVLLR	3	93.3	1	34.23	0	N/D
716	RHPEYAVSVLLR	7	90.55	2	46.35	0	N/D
718	RHPEYAVSVLLR	3	114.84	1	44.23	0	N/D
720	RHPEYAVSVLLR	3	101.23	1	54.12	0	N/D
728	RHPEYAVSVLLR	2	109.12	0	N/D	0	N/D
730	RHPEYAVSVLLR	2	109.53	0	N/D	0	N/D
734	RHPEYAVSVLLR	2	120.96	0	N/D	0	N/D
746	RHPEYAVSVLLR	2	117.62	0	N/D	0	N/D
754	RHPEYAVSVLLR	3	76.57	2	46.49	1	4.46
774	KQTALVELLK	5	82.33	2	55.65	1	2.24
774	QTALVELLK	4	89.77	2	34.43	1	3.29
776	QTALVELLK	4	89.77	2	63.93	1	2.36
778	QTALVELLK	5	105.87	2	63.79	0	N/D
779	QTALVELLK	2	64.57	2	64.57	0	N/D
782	QTALVELLK	5	103.56	2	64.33	0	N/D
784	QTALVELLK	4	88.73	2	64.03	0	N/D
786	QTALVELLK	5	103.9	2	63.1	0	N/D
806	LGEYGFQNALIVR	5	74.5	2	63.74	0	N/D
810	LGEYGFQNALIVR	11	78.91	3	50.43	0	N/D
812	LGEYGFQNALIVR	7	67.56	3	39.26	0	N/D

814	LGEYGFQNALIVR	8	63.95	5	49.55	0	N/D
816	LGEYGFQNALIVR	10	73.12	6	47.76	0	N/D
822	LGEYGFQNALIVR	10	72.95	3	50.07	0	N/D
824	LGEYGFQNALIVR	5	73.93	3	46.73	0	N/D
826	LGEYGFQNALIVR	5	73.46	3	49.73	0	N/D
828	LGEYGFQNALIVR	6	67.95	3	49.23	0	N/D
952	RHPYFYAPELLYYANK	13	58.73	3	48.99	0	N/D
954	RHPYFYAPELLYYANK	13	58.91	6	37.83	0	N/D
956	RHPYFYAPELLYYANK	13	58.8	5	37.75	0	N/D
958	RHPYFYAPELLYYANK	10	62.7	5	37.63	0	N/D
960	RHPYFYAPELLYYANK	14	61.61	3	34.31	0	N/D
962	RHPYFYAPELLYYANK	14	61.09	5	37.61	0	N/D
964	RHPYFYAPELLYYANK	14	58.25	5	37.24	0	N/D
966	RHPYFYAPELLYYANK	14	61.06	5	37.51	0	N/D
968	RHPYFYAPELLYYANK	14	61.16	5	37.22	0	N/D
970	RHPYFYAPELLYYANK	14	61.19	5	37.4	0	N/D
972	RHPYFYAPELLYYANK	14	61.17	5	37.37	0	N/D
974	RHPYFYAPELLYYANK	12	61.4	5	37.41	0	N/D
976	RHPYFYAPELLYYANK	11	58.13	5	37.7	0	N/D
978	RHPYFYAPELLYYANK	11	53.89	5	37.83	0	N/D
980	RHPYFYAPELLYYANK	12	57.37	5	37.46	0	N/D
982	RHPYFYAPELLYYANK	10	59.7	5	37.41	0	N/D
984	RHPYFYAPELLYYANK	10	66.45	4	38.63	0	N/D
986	RHPYFYAPELLYYANK	10	66.82	4	44.01	0	N/D
988	RHPYFYAPELLYYANK	9	64.99	3	42.79	0	N/D
990	RHPYFYAPELLYYANK	10	66.52	3	42.48	0	N/D
average absolute error (ppm)			**85.03**		**48.02**		**4.32**

Supplementary data

Table 2. Average mass measurement errors of the identified peptides for tryptic digestion of BSA during a multiplexed LC-CID-FTICR-MS separation (after COFI)

		mass tol. = 0.1 Da		mass tol. = 0.02 Da		mass tol. = 0.01 Da		
File #	Sequence	No. of fragment	average absolute error (ppm)	No. of fragment	average absolute error (ppm)	No. of fragment	average absolute error (ppm)	frequency shift (*Hz*)
484	FKDLGEEHFK	11	5.07	11	5.07	10	4.66	21.991
486	FKDLGEEHFK	8	4.1	8	4.1	7	3.11	23.297
488	FKDLGEEHFK	12	3.64	12	3.64	12	3.64	22.27
490	FKDLGEEHFK	11	10.31	10	4.18	10	4.18	22.094
492	FKDLGEEHFK	10	3.86	10	3.86	10	3.86	21.93
494	FKDLGEEHFK	8	1.34	8	1.34	8	1.34	22.496
498	DAFLGSFLYEYSR	3	17.75	2	6.65	1	1.15	23.372
498	FKDLGEEHFK	2	3.62	2	3.62	2	3.62	23.372
500	DAFLGSFLYEYSR	3	15.84	2	6.61	1	2.18	22.753
506	FKDLGEEHFK	3	3.5	3	3.5	3	3.5	22.066
508	FKDLGEEHFK	2	6.78	2	6.78	1	3.2	23.627
518	FKDLGEEHFK	2	3.18	2	3.18	2	3.18	22.849
528	HLVDEPQNLIK	8	2.29	8	2.29	8	2.29	22.554
530	HLVDEPQNLIK	11	1.9	11	1.9	11	1.9	22.323
532	HLVDEPQNLIK	10	1.29	10	1.29	10	1.29	22.793
534	HLVDEPQNLIK	11	2.59	11	2.59	11	2.59	22.2
536	HLVDEPQNLIK	11	1.3	11	1.3	11	1.3	22.489
538	HLVDEPQNLIK	10	2.39	10	2.39	10	2.39	22.183
538	LVVSTQTALA	2	2.41	2	2.41	2	2.41	22.183
538	YLYEIAR	2	3.35	2	3.35	2	3.35	22.183
540	HLVDEPQNLIK	10	1.27	10	1.27	10	1.27	22.351
540	LVVSTQTALA	3	1.88	3	1.88	3	1.88	22.351
540	YLYEIAR	2	2.34	2	2.34	2	2.34	22.351
542	HLVDEPQNLIK	7	2.69	7	2.69	7	2.69	22.368
542	YLYEIAR	3	4.23	3	4.23	3	4.23	22.368
544	HLVDEPQNLIK	7	3.3	7	3.3	7	3.3	21.669
544	YLYEIAR	3	5.34	3	5.34	3	5.34	21.669
546	HLVDEPQNLIK	6	0.93	6	0.93	6	0.93	22.072
546	YLYEIAR	3	1.84	3	1.84	3	1.84	22.072
548	HLVDEPQNLIK	5	1.94	5	1.94	5	1.94	21.884
548	YLYEIAR	3	4.08	3	4.08	3	4.08	21.884

552	**HLVDEPQNLIK**	**4**	**23.18**	**1**	**1.15**	**1**	**1.15**	**28.845**
552	**YLYEIAR**	**3**	**24.02**	**1**	**2.35**	**1**	**2.35**	**28.845**
554	YLYEIAR	2	2.33	2	2.33	2	2.33	22.9
556	HLVDEPQNLIK	2	5.2	2	5.2	1	2.62	22.251
556	LKHLVDEPQNLIK	4	15.97	3	4.38	2	3	22.251
558	HLVDEPQNLIK	2	3.08	2	3.08	2	3.08	22.475
558	LKHLVDEPQNLIK	4	15.14	3	2.93	3	2.93	22.475
558	YLYEIAR	2	2.6	2	2.6	2	2.6	22.475
564	HLVDEPQNLIK	4	1.57	4	1.57	4	1.57	22.251
566	**YLYEIAR**	**2**	**76.5**	**0**	**N/D**	**0**	**N/D**	**0**
568	KVPQVSTPTLVEVSR	11	1.57	11	1.57	11	1.57	22.034
570	KVPQVSTPTLVEVSR	11	1.43	11	1.43	11	1.43	23.653
572	KVPQVSTPTLVEVSR	12	4	11	1.18	11	1.18	22.763
574	KVPQVSTPTLVEVSR	12	5.9	12	5.9	6	4.04	21.246
576	KVPQVSTPTLVEVSR	9	1.57	9	1.57	9	1.57	23.603
578	KVPQVSTPTLVEVSR	12	1.14	12	1.14	12	1.14	22.87
580	KVPQVSTPTLVEVSR	12	1.44	12	1.44	12	1.44	22.182
582	KVPQVSTPTLVEVSR	11	1.53	11	1.53	11	1.53	22.667
584	KVPQVSTPTLVEVSR	9	1.56	9	1.56	9	1.56	22.39
586	KVPQVSTPTLVEVSR	11	1.43	11	1.43	11	1.43	21.891
588	KVPQVSTPTLVEVSR	8	0.95	8	0.95	8	0.95	23.1
590	KVPQVSTPTLVEVSR	8	2.55	8	2.55	8	2.55	21.909
592	KVPQVSTPTLVEVSR	7	1.37	7	1.37	7	1.37	21.919
594	KVPQVSTPTLVEVSR	6	1.82	6	1.82	6	1.82	21.758
596	KVPQVSTPTLVEVSR	6	2.52	6	2.52	6	2.52	21.491
598	KVPQVSTPTLVEVSR	4	1.45	4	1.45	4	1.45	22.216
602	KVPQVSTPTLVEVSR	4	1.59	4	1.59	4	1.59	21.711
632	**HLVDEPQNLIK**	**2**	**14.91**	**0**	**N/D**	**0**	**N/D**	**19.693**
636	HLVDEPQNLIK	2	10.03	2	9.33	1	1.03	22.477
642	LVNELTEFAK	4	1.2	4	1.2	4	1.2	22.355
644	HLVDEPQNLIK	3	14.65	1	1.17	1	1.17	21.852
644	LVNELTEFAK	7	10.18	6	2.58	6	2.58	21.852
648	LVNELTEFAK	6	2.31	6	2.31	6	2.31	22.348
650	LVNELTEFAK	7	3.32	7	3.32	6	1.43	22.109
652	**LVNELTEFAK**	**3**	**57.02**	**0**	**N/D**	**0**	**N/D**	42.038
654	LVNELTEFAK	5	1.31	5	1.31	5	1.31	22.257
656	LVNELTEFAK	6	1.41	6	1.41	6	1.41	21.838
658	LVNELTEFAK	6	11.47	5	1.33	5	1.33	22.215
660	LVNELTEFAK	6	13.75	5	4.48	5	4.48	21.352
662	**LVNELTEFAK**	**6**	**25.1**	**2**	**13.21**	**0**	**N/D**	17.487
664	LVNELTEFAK	5	1.22	5	1.22	5	1.22	22.207
666	LVNELTEFAK	5	1.79	5	1.79	5	1.79	21.909
668	LVNELTEFAK	5	10.2	4	2.16	4	2.16	21.583
670	LVNELTEFAK	4	4.39	4	4.39	4	4.39	20.991
672	LVNELTEFAK	4	6.06	4	6.06	3	5.05	20.698
674	KQTALVELLK	10	2.02	10	2.02	10	2.02	22.222
674	LVNELTEFAK	4	1.95	4	1.95	4	1.95	22.222
676	KQTALVELLK	10	0.98	10	0.98	10	0.98	22.974
676	RHPEYAVSVLLR	3	1.15	3	1.15	3	1.15	22.974
678	KQTALVELLK	8	4.99	8	4.99	8	4.99	22.439

678	LVNELTEFAK	4	5.59	4	5.59	4	5.59	22.439
678	RHPEYAVSVLLR	10	6.65	9	3.47	9	3.47	22.439
680	KQTALVELLK	9	1.49	9	1.49	9	1.49	22.862
680	RHPEYAVSVLLR	10	2.21	10	2.21	10	2.21	22.862
682	KQTALVELLK	6	3.06	6	3.06	6	3.06	22.025
682	RHPEYAVSVLLR	10	2.29	10	2.29	10	2.29	22.025
684	KQTALVELLK	6	1.82	6	1.82	6	1.82	22.524
684	RHPEYAVSVLLR	8	1.79	8	1.79	8	1.79	22.524
686	KQTALVELLK	9	2.43	9	2.43	9	2.43	22.545
686	RHPEYAVSVLLR	8	1.42	8	1.42	8	1.42	22.545
688	KQTALVELLK	7	4.44	7	4.44	6	3.62	21.717
688	RHPEYAVSVLLR	11	4.26	11	4.26	9	3.37	21.717
690	KQTALVELLK	3	5.86	3	5.86	3	5.86	21.937
690	LVNELTEFAK	3	3.33	3	3.33	3	3.33	21.937
690	RHPEYAVSVLLR	9	4.14	9	4.14	8	3.45	21.937
692	KQTALVELLK	8	4.58	8	4.58	8	4.58	21.962
692	RHPEYAVSVLLR	8	3.28	8	3.28	7	2.75	21.962
694	RHPEYAVSVLLR	11	2.69	11	2.69	11	2.69	21.927
698	KQTALVELLK	7	3.24	7	3.24	7	3.24	22.075
698	RHPEYAVSVLLR	8	2	8	2	8	2	22.075
700	**RHPEYAVSVLLR**	**4**	**49.53**	**0**	**N/D**	**0**	**N/D**	**0**
702	LVNELTEFAK	2	3.55	2	3.55	2	3.55	22.171
702	RHPEYAVSVLLR	9	2.65	9	2.65	9	2.65	22.171
704	KQTALVELLK	9	3.92	9	3.92	9	3.92	22.019
704	RHPEYAVSVLLR	9	3.25	9	3.25	8	2.37	22.019
706	KQTALVELLK	2	2.66	2	2.66	2	2.66	22.391
706	RHPEYAVSVLLR	6	9.8	5	3.75	4	2.95	22.391
712	RHPEYAVSVLLR	3	16.31	2	4.41	2	4.41	22.288
714	**RHPEYAVSVLLR**	**4**	**46.09**	**0**	**N/D**	**0**	**N/D**	14.513
716	HPEYAVSVLLR	3	3.21	3	3.21	3	3.21	22.416
716	RHPEYAVSVLLR	7	3.12	7	3.12	7	3.12	22.416
718	RHPEYAVSVLLR	3	5.69	3	5.69	3	5.69	21.314
720	RHPEYAVSVLLR	3	3.38	3	3.38	3	3.38	24.587
728	RHPEYAVSVLLR	2	4.8	2	4.8	2	4.8	21.958
730	RHPEYAVSVLLR	2	3.78	2	3.78	2	3.78	21.555
734	**RHPEYAVSVLLR**	**2**	**38.28**	**0**	**N/D**	**0**	**N/D**	30.288
746	RHPEYAVSVLLR	2	2.21	2	2.21	2	2.21	21.9
754	**RHPEYAVSVLLR**	**2**	**46.49**	**0**	**N/D**	**0**	**N/D**	0
772	QTALVELLK	2	5.92	2	5.92	1	1.4	20.743
774	KQTALVELLK	6	3.16	6	3.16	6	3.16	21.664
774	QTALVELLK	4	3.12	4	3.12	4	3.12	21.664
776	QTALVELLK	4	3.18	4	3.18	4	3.18	21.648
778	QTALVELLK	5	2.45	5	2.45	5	2.45	22.296
780	QTALVELLK	5	1.4	5	1.4	5	1.35	22.276
782	QTALVELLK	5	1.35	5	1.35	4	2.47	22.239
784	QTALVELLK	4	2.47	4	2.47	2	1.44	21.573
786	QTALVELLK	5	2.72	5	2.72	5	2.72	21.804
806	LGEYGFQNALIVR	7	1.6	7	1.6	7	1.6	22.115
810	LGEYGFQNALIVR	15	4.3	14	2.65	13	2.3	22.325
812	LGEYGFQNALIVR	9	3.67	9	3.67	8	3.11	21.835

814	LGEYGFQNALIVR	10	1.05	10	1.05	10	1.05	22.435
816	LGEYGFQNALIVR	13	3.15	12	1.46	12	1.46	22.882
822	LGEYGFQNALIVR	12	3.47	11	1.58	11	1.58	22.407
824	**LGEYGFQNALIVR**	**3**	**44.56**	**0**	**N/D**	**0**	**N/D**	1.2102
826	**LGEYGFQNALIVR**	**6**	**20.2**	**2**	**10.13**	**1**	**1.98**	16.871
828	LGEYGFQNALIVR	7	2.81	7	2.81	7	2.81	21.492
952	RHPYFYAPELLYYANK	16	1.82	16	1.82	16	1.82	21.781
954	RHPYFYAPELLYYANK	17	2.15	17	2.15	17	2.15	21.814
956	RHPYFYAPELLYYANK	16	1.72	16	1.72	16	1.72	21.881
958	RHPYFYAPELLYYANK	11	2.93	11	2.93	11	2.93	21.354
960	RHPYFYAPELLYYANK	17	2	17	2	17	2	21.784
962	RHPYFYAPELLYYANK	16	1.3	16	1.3	16	1.3	21.797
964	RHPYFYAPELLYYANK	16	2.03	16	2.03	15	2.13	21.874
966	HPYFYAPELLYYANK	17	1.1	17	1.1	17	1.1	21.878
968	HPYFYAPELLYYANK	16	1.75	15	1.2	15	1.2	21.883
970	HPYFYAPELLYYANK	16	2.31	16	2.31	15	1.99	21.6
972	HPYFYAPELLYYANK	15	1.68	15	1.68	15	1.68	21.721
974	HPYFYAPELLYYANK	12	2.15	12	2.15	12	2.15	21.744
976	HPYFYAPELLYYANK	12	2.1	12	2.1	12	2.1	21.797
978	HPYFYAPELLYYANK	13	2.16	13	2.16	13	2.16	21.652
980	HPYFYAPELLYYANK	12	2.5	12	2.5	12	2.5	21.422
982	HPYFYAPELLYYANK	11	1.86	11	1.86	11	1.86	21.653
984	HPYFYAPELLYYANK	10	1.03	10	1.03	10	1.03	21.746
986	RHPYFYAPELLYYANK	10	1.8	10	1.8	10	1.8	21.546
988	HPYFYAPELLYYANK	9	1.1	9	1.1	9	1.1	22.281
990	HPYFYAPELLYYANK	10	4.1	10	4.1	9	3.58	20.677
	average absolute error (ppm)		**6.43**		**2.89**		**2.49**	