

Supplemental Material

Table S1. Identified cross-links in rHDL.

rHDL-2-100 Replicate1										
Peptide a	Peptide b	CL site a	CL site b	APOA1 Pos1	APOA1 Pos2	Mr	Mz	z	Id-Score	Type
DYVSQFEGSALGK	VSFLSALEEYTKK	a7	b12	34	238	2895.448	724.87	4	28.52	intra
QLNLKLLDNWDSVT STFSK	DYVSQFEGSALGK	a5	b7	45	34	3589.795	1197.606	3	50	intra
EQLGPVTQEFWDNL EK	VKDLATVYVDVLK	a15	b2	76	12	3375.765	1126.263	3	39.32	intra
AKVQPYLDDFQK	THLAPYSDEL R	a2	b8	96	168	2733.376	547.683	5	45.74	inter
AKVQPYLDDFQK	THLAPYSDEL R	a2	b9	96	169	2733.378	912.134	3	45.28	inter
AKVQPYLDDFQKK	THLAPYSDEL R	a2	b8	96	168	2861.473	573.302	5	38.66	inter
AKVQPYLDDFQKK	LSPLGEEMRDR	a2	b6	96	146	2862.474	716.626	4	26.69	inter
KWQEEMEL YR	AELQEGAR	a1	b2	107	125	2265.084	567.279	4	44.26	inter
KWQEEMEL YR	LSPLGEEMR	a1	b7	107	147	2423.163	808.729	3	31.73	inter
QKLHELQEK	AELQEGAR	a2	b2	133	125	2006.054	502.521	4	38.61	inter
QKLHELQEK	WQEEMEL YR	a2	b4	133	111	2416.184	605.054	4	29.17	inter
QKLHELQEK	WQEEMEL YR	a2	b3	133	110	2416.175	806.4	3	26.66	inter
QKLHELQEK	AELQEGAR	a2	b5	133	128	2006.054	502.521	4	37.25	intra
LHELQEKLSPLGEEM R	AELQEGAR	a7	b2	140	125	2762.403	553.488	5	39.51	inter

Cross-linking and MS/MS reveals multiple registries in APOA1

LSPLGEEMR	QKVEPLR	a7	b2	147	118	1881.015	628.013	3	32.11	inter
ATEHLSTLSEK	AKPALEDLR	a3	b2	198	208	2208.176	553.052	4	38.75	intra
VSFLSALEEYTK	AKPALEDLR	a9	b2	235	208	2379.269	595.825	4	31.54	intra
rHDL-2-100 Replicate2										
VKDLATVYVDVLK	VSFLSALEEYTK	a2	b9	12	235	2829.536	944.187	3	33.53	intra
DLATVYVDVLKDSGR	LLDNWDSVTSTFSK	a11	b3	23	48	3243.635	1082.219	3	25.77	intra
DYVSQFEGSALGK	VSFLSALEEYTKK	a7	b12	34	238	2895.461	966.161	3	33.65	intra
QLNLKLLDNWDSVT STFSK	DYVSQFEGSALGK	a5	b7	45	34	3589.812	1197.612	3	34.59	intra
LREQLGPVTQEFWD NLEK	VKDLATVYVDVLK	a17	b2	76	12	3644.945	912.244	4	38.74	intra
AKVQPYLDDFQK	THLAPYSDELRL	a2	b9	96	169	2733.379	912.134	3	33.14	inter
AKVQPYLDDFQK	THLAPYSDELRL	a2	b8	96	168	2733.374	684.351	4	32.96	inter
AKVQPYLDDFQKK	THLAPYSDELRL	a2	b9	96	169	2861.471	954.831	3	32.13	inter
AKVQPYLDDFQK	LSPLGEEMR	a2	b7	96	147	2463.253	822.092	3	28.44	inter
KWQEEMELYL	AHVDALR	a1	b4	107	157	2173.078	725.367	3	33.08	inter
KWQEEMELYL	AELQEGAR	a1	b2	107	125	2265.089	1133.552	2	30.46	inter
KWQEEMELYL	QKLHELQEK	a5	b2	111	133	2544.281	637.078	4	24.64	inter
QKLHELQEK	AELQEGAR	a2	b2	133	125	2006.052	669.692	3	26.15	inter
LHELQEKLSPLGEEM R	AELQEGAR	a7	b2	140	125	2762.406	691.609	4	43.79	inter
LSPLGEEMR	QKVEPLR	a7	b2	147	118	1881.015	471.262	4	29.51	inter
LAEYHAKATEHLSTL SEK	LREQLGPVTQEFW DNLEK	a7	b11	195	70	4210.142	1053.543	4	32.97	inter

Cross-linking and MS/MS reveals multiple registries in APOA1

LAEYHAKATEHLSTL SEK	ETEGLR	a7	b1	195	78	2712.372	679.101	4	27.28	inter
LAEYHAKATEHLSTL SEK	ETEGLR	a7	b3	195	80	2712.38	905.134	3	26.2	inter
ATEHLSTLSEK	AKPALEDLR	a3	b2	198	208	2208.175	442.643	5	31.34	intra
QGLLPVLESFK	AKPALEDLR	a8	b2	223	208	2223.269	556.825	4	29.55	intra
VSFLSALEEYTKKLN TQ	ATEHLSTLSEK	a13	b3	239	198	3166.622	634.332	5	21.59	intra
rHDL-2-100 Replicate3										
Peptide a	Peptide b	CL site a	CL site b	APOA1 Pos1	APOA1 Pos2	Mr	Mz	z	Id-Score	Type
VKDLATVYVDVLK	ETEGLR	a2	b1	12	78	2147.203	716.742	3	36.51	intra
VKDLATVYVDVLKDS GR	LLDNWDSVTSTFSK	a13	b3	23	48	3470.814	868.711	4	33.47	intra
DLATVYVDVLKDSGR	LLDNWDSVTSTFSK	a11	b3	23	48	3243.643	1082.222	3	34.8	intra
DYVSQFEGSALGK	VSFLSALEEYTKK	a7	b12	34	238	2895.464	966.163	3	32.22	intra
AKVQPYLDDFQKK	THLAPYSDELRL	a2	b8	96	168	2861.491	716.38	4	34.48	inter
AKVQPYLDDFQKK	LSPLGEEMR	a2	b7	96	147	2591.354	648.846	4	21.53	inter
AKVQPYLDDFQKK	LSPLGEEMR	a2	b6	96	146	2591.354	648.846	4	20.15	inter
KWQEEMELYSR	AELQEGAR	a1	b2	107	125	2265.093	567.281	4	58.21	inter
KWQEEMELYSR	QKLHELQEK	a4	b2	110	133	2544.285	509.865	5	30.66	inter
KWQEEMELYSR	QKLHELQEK	a5	b2	111	133	2544.291	509.866	5	32.08	inter
QKLHELQEKLSPLGE EMR	AELQEGAR	a9	b2	140	125	3018.569	755.65	4	29.01	inter

Cross-linking and MS/MS reveals multiple registries in APOA1

LSPLGEEMR	QKVEPLR	a6	b2	146	118	1881.026	471.264	4	28.49	inter
LAEYHAKATEHLSTL SEK	ETEGLR	a7	b1	195	78	2712.39	453.073	6	31.6	inter
QGLLPVLESFKVSFL SALEEYTKK	AKPALEDLR	a8	b2	223	208	3719.047	620.849	6	24.79	intra
QGLLPVLESFKVSFL SALEEYTK	DYVSQFEGSALGK	a11	b7	226	34	3979.085	995.779	4	23.88	intra
rHDL-2-100 Replicate4										
Peptide a	Peptide b	CL site a	CL site b	APOA1 Pos1	APOA1 Pos2	Mr	Mz	z	Id-Score	Type
DLATVYVDVLKDSGR	LLDNWDSVTSTFSK	a11	b3	23	48	3243.64	1082.221	3	40.67	intra
QLNLKLLDNWDSVT STFSK	DYVSQFEGSALGK	a5	b7	45	34	3589.809	1197.611	3	37.87	intra
EQLGPVTQEFWDNL EK	VKDLATVYVDVLK	a15	b2	76	12	3375.775	1126.266	3	26.86	intra
AKVQPYLDDFQK	THLAPYSDELRL	a2	b9	96	169	2733.386	684.354	4	40.36	inter
AKVQPYLDDFQK	THLAPYSDELRL	a2	b8	96	168	2733.389	684.355	4	40.46	inter
AKVQPYLDDFQK	LSPLGEEMR	a2	b6	96	146	2463.253	616.821	4	31.17	inter
KWQEEMELYLRL	AHVDALRL	a1	b4	107	157	2173.078	725.367	3	41.38	inter
QKVEPLRAELQEGAR	KWQEEMELYLRL	a9	b1	125	107	3115.569	779.9	4	23.11	inter
QKLHELQEK	AELQEGAR	a2	b2	133	125	2006.062	402.22	5	31.66	inter
QKLHELQEK	WQEEMELYLRL	a2	b3	133	110	2416.188	484.245	5	27.88	inter

Cross-linking and MS/MS reveals multiple registries in APOA1

LHELQEKLSPLGEEM RDR	AELQEGAR	a7	b2	140	125	3033.541	607.716	5	35.07	inter
LSPLGEEMR	QKVEPLR	a7	b2	147	118	1881.022	471.263	4	31.68	inter
LAEYHAKATEHLSTL SEK	ETEGLR	a7	b3	195	80	2712.376	543.483	5	27.16	inter
LAEYHAKATEHLSTL SEK	EQLGPVTQEFWDN LEK	a7	b9	195	70	3940.965	986.249	4	26.2	inter
ATEHLSTLSEK	AKPALEDLR	a3	b2	198	208	2208.179	737.068	3	41.57	intra
QGLLPVLESFKVSFL SALEEYTK	ATEHLSTLSEK	a11	b10	226	205	3794.04	759.816	5	30.36	intra
rHDL-2-80 replicate 1										
Peptide a	Peptide b	CL site a	CL site b	APOA1 Pos1	APOA1 Pos2	Mr	Mz	z	Id-Score	Type
DLATVYVDVLKDSGR	DYVSQFEGSALGK	a11	b7	23	34	3031.512	1011.512	3	40.16	intra
DLATVYVDVLKDSGR	DYVSQFEGSALGK	a11	b1	23	28	3031.517	758.887	4	38.41	intra
DYVSQFEGSALGKQ LNLK	VSFLSALEEYTK	a13	b8	40	234	3363.733	1122.252	3	42.41	intra
EQLGPVTQEFWDNL EK	VKDLATVYVDVLK	a12	b2	73	12	3375.784	844.954	4	28.32	intra
AKVQPYLDDFQK	THLAPYSDEL R	a2	b9	96	169	2733.38	912.135	3	45.81	inter
AKVQPYLDDFQK	THLAPYSDEL R	a2	b8	96	168	2733.379	547.684	5	45.18	inter
AKVQPYLDDFQKK	DLEEVK	a2	b3	96	91	2292.195	574.057	4	33.74	intra
AKVQPYLDDFQK	LSPLGEEMR	a2	b7	96	147	2463.245	822.089	3	32.3	inter
KWQEEMEL YR	AELQEGAR	a1	b2	107	125	2265.088	567.28	4	45.19	inter
KWQEEMEL YR	LSPLGEEMR	a1	b7	107	147	2423.168	808.731	3	31.61	inter
QKLHELQEK	DLEEVK	a2	b1	133	89	1864.991	622.671	3	34.19	intra
QKLHELQEK	WQEEMEL YR	a2	b4	133	111	2416.185	484.245	5	32.54	inter
LHELQEK	QKVEPLR	a6	b2	139	118	1745.978	437.502	4	30.01	intra

Cross-linking and MS/MS reveals multiple registries in APOA1

LHELQEKLSPLGEEM R	AELQEGAR	a7	b2	140	125	2762.405	691.609	4	40.2	inter
LHELQEKLSPLGEEM RDR	AELQEGAR	a7	b2	140	125	3033.531	759.39	4	29.31	inter
LSPLGEEMR	QKVEPLR	a7	b2	147	118	1881.015	628.013	3	32.85	inter
LAEYHAKATEHLSTL SEK	ETEGLR	a7	b1	195	78	2712.374	679.101	4	33.28	inter
LAEYHAKATEHLSTL SEK	EQLGPVTQEFWDN LEK	a7	b9	195	70	3940.955	657.834	6	30.11	inter
QGLLPVLESFKVSFL SALEEYTK	ATEHLSTLSEK	a11	b3	226	198	3794.022	759.812	5	34.81	intra
QGLLPVLESFKVSFL SALEEYTK	AKPALEDLR	a11	b7	226	213	3590.982	898.753	4	28.7	intra
VSFLSALEEYTK	AKPALEDLR	a9	b2	235	208	2379.271	595.826	4	33.08	intra
rHDL-2-80 replicate 2										
Peptide a	Peptide b	CL site a	CL site b	APOA1 Pos1	APOA1 Pos2	Mr	Mz	z	Id-Score	Type
VKDLATVYVDVLK	ETEGLR	a2	b1	12	78	2147.185	716.736	3	34.42	intra
VKDLATVYVDVLK	ETEGLR	a2	b3	12	80	2147.185	537.804	4	31.59	intra
VKDLATVYVDVLKDS GR	DYVSQFEGSALGK GR	a13	b1	23	28	3258.679	815.678	4	50.44	intra
DLATVYVDVLKDSGR	LLDNWDSVTSTFSK	a11	b6	23	51	3243.631	1082.218	3	38.95	intra
DLATVYVDVLKDSGR	DYVSQFEGSALGK	a11	b1	23	28	3031.517	758.887	4	38.41	intra
QLNLKLLDNWDSVT STFSK	DYVSQFEGSALGK	a5	b7	45	34	3589.799	1197.607	3	52.67	intra
AKVQPYLDDFQKK	THLAPYSDEL R	a2	b8	96	168	2861.473	716.376	4	39.5	inter
AKVQPYLDDFQKK	THLAPYSDEL R	a2	b9	96	169	2861.477	716.377	4	33.64	inter
AKVQPYLDDFQK	LSPLGEEMR	a2	b6	96	146	2463.246	822.09	3	31.34	inter
AKVQPYLDDFQKK	LSPLGEEMRDR	a2	b6	96	146	2862.475	573.503	5	25.01	inter
KWQEEMEL YR	VQPYLDDFQK	a1	b6	107	102	2644.263	662.074	4	38.05	intra
KWQEEMEL YR	LSPLGEEMR	a1	b6	107	146	2423.164	606.799	4	34	inter
QKVEPLRAELQEGA R	LSPLGEEMR	a2	b7	118	147	2735.433	684.866	4	28.65	inter

Cross-linking and MS/MS reveals multiple registries in APOA1

QKLHELQEK	AELQEGAR	a2	b2	133	125	2006.055	502.522	4	37.16	inter
QKLHELQEK	AELQEGAR	a2	b5	133	128	2006.056	502.522	4	36.75	intra
QKLHELQEK	WQEEMELYR	a2	b3	133	110	2416.191	605.055	4	32.66	inter
QKLHELQEKLSPLGE EMR	AELQEGAR	a9	b2	140	125	3018.558	755.647	4	31.69	inter
LAEYHAKATEHLSTL SEK	ETEGLR	a7	b3	195	80	2712.376	543.483	5	33.5	inter
LAEYHAKATEHLSTL SEK	LREQLGPVTQEFW DNLEK	a7	b14	195	73	4210.128	843.033	5	30.92	inter
ATEHLSTLSEK	AKPALEDLR	a10	b2	205	208	2208.177	737.067	3	40.78	intra
ATEHLSTLSEKAKPA LEDLR	AKPALEDLR	a11	b7	206	213	3201.739	1068.254	3	27.44	intra
AKPALEDLR	LAEYHAK	a2	b3	208	191	1823.989	457.005	4	36.98	intra
QGLLPVLESFKVSFL SALEEYTK	ATEHLSTLSEK	a11	b10	226	205	3794.029	759.814	5	34.37	intra
VSFLSALEEYTK	AKPALEDLR	a8	b2	234	208	2379.279	794.101	3	37.6	intra
rHDL-2-120 replicate 1										
Peptide a	Peptide b	CL site a	CL site b	APOA1 Pos1	APOA1 Pos2	Mr	Mz	z	Id-Score	Type
DYVSQFEGSALGK	QKLHELQEK	a1	b2	28	133	2533.274	845.433	3	31.86	intra
QLNLKLLDNWDSVT STFSK	DYVSQFEGSALGK	a5	b7	45	34	3589.79	898.455	4	29.44	intra
LREQLGPVTQEFWD NLEKETEGLR	QEMSKDLEEVK	a21	b5	80	88	4203.072	701.52	6	32.83	intra
AKVQPYLDDFQK	THLAPYSDELRL	a2	b9	96	169	2733.37	547.682	5	47.65	inter
AKVQPYLDDFQK	THLAPYSDELRL	a2	b8	96	168	2733.367	684.349	4	39.57	inter
AKVQPYLDDFQK	DLEEVK	a2	b3	96	91	2164.103	542.034	4	37.96	intra
AKVQPYLDDFQKK	LSPLGEEMRDR	a2	b6	96	146	2862.471	573.502	5	26.32	inter

Cross-linking and MS/MS reveals multiple registries in APOA1

KWQEEMELYSR	AELQEGAR	a1	b2	107	125	2265.079	567.278	4	39.87	inter
WQEEMELYSR	QKVEPLR	a6	b2	113	118	2133.063	534.274	4	32.41	intra
QKVEPLRAELQEGAR	LSPLGEEMR	a2	b7	118	147	2735.436	684.867	4	27.36	inter
AELQEGAR	QKVEPLR	a2	b2	125	118	1722.935	575.319	3	32.27	intra
QKLHELQEK	AELQEGAR	a2	b5	133	128	2006.049	402.218	5	38.34	intra
QKLHELQEK	AELQEGAR	a2	b2	133	125	2006.05	502.52	4	36.09	inter
LHELQEK	QKVEPLR	a6	b2	139	118	1745.977	873.996	2	29.44	intra
LHELQEKLSPLGEEMR	AELQEGAR	a7	b2	140	125	2762.4	691.608	4	39.64	inter
LSPLGEEMR	QKLHELQEK	a7	b2	147	133	2164.126	722.383	3	29.19	intra
LSPLGEEMR	QKVEPLR	a7	b2	147	118	1881.009	471.26	4	29.19	inter
LEALKENGGAR	LAEYHAK	a5	b3	182	191	1969.034	657.353	3	30.72	intra
ATEHLSTLSEK	AKPALEDLR	a3	b2	198	208	2208.168	553.05	4	35.82	intra
ATEHLSTLSEK	LEALKENGGAR	a3	b5	198	182	2353.227	589.314	4	24.55	intra
rHDL-2-120 replicate 2										
Peptide a	Peptide b	CL site a	CL site b	APOA1 Pos1	APOA1 Pos2	Mr	Mz	z	Id-Score	Type
DYVSQFEGSALGK	QKLHELQEK	a1	b2	28	133	2533.276	845.433	3	37.17	intra
LREQLGPVTQEFWD NLEKETEGLR	QEMSKDLEEVK	a19	b5	78	88	4203.081	1051.778	4	23.58	intra
LREQLGPVTQEFWD NLEKETEGLR	QEMSKDLEEVK	a21	b5	80	88	4203.081	701.521	6	31.12	intra
AKVQPYLDDFQK	THLAPYSDELRL	a2	b9	96	169	2733.372	912.132	3	44.9	inter

Cross-linking and MS/MS reveals multiple registries in APOA1

AKVQPYLDDFQKK	LSPLGEEMRDR	a2	b6	96	146	2862.468	716.625	4	23.78	inter
QKVEPLRAELQEGAR	LSPLGEEMR	a2	b6	118	146	2735.438	548.095	5	22.46	inter
AELQEGAR	QKVEPLR	a2	b2	125	118	1722.935	575.32	3	35.61	intra
QKLHELQEK	AELQEGAR	a2	b2	133	125	2006.052	502.521	4	40.96	inter
QKLHELQEK	AELQEGAR	a2	b5	133	128	2006.05	669.691	3	34.95	intra
QKLHELQEK	WQEEMELR	a2	b3	133	110	2416.18	605.053	4	22.14	intra
LHELQEK	QKVEPLR	a6	b2	139	118	1745.977	583	3	34.91	intra
LHELQEKLSPLGEEMR	AELQEGAR	a7	b2	140	125	2762.395	691.607	4	39.75	inter
LSPLGEEMR	QKLHELQEK	a7	b2	147	133	2164.127	722.384	3	31.2	intra
LAARLEALKENGGAR	THLAPYSDELRR	a9	b9	182	169	3134.666	627.941	5	25.39	intra
ATEHLSTLSEK	LEALKENGGAR	a3	b5	198	182	2353.223	589.314	4	24.95	intra
ATEHLSTLSEK	AKPALEDLR	a10	b2	205	208	2208.171	553.05	4	35.08	intra
QGLLPVLESFKVSFL SALEEYTK	AKPALEDLR	a11	b7	226	213	3590.979	898.753	4	24.76	intra

Table S2. Identified cross-links in human HDL

Replicate 1									
Peptide a	Peptide b	CL site a	CL site b	APOA1 Pos1	APOA1 Pos2	Mr	Mz	z	Id-Score
VKDLATVYVDVLKDSGR	DYVSQFEGSALGK	a13	b1	23	28	3258.677	815.677	4	40.89
DLATVYVDVLKDSGR	DYVSQFEGSALGK	a11	b1	23	28	3031.519	1011.514	3	26.78
QLNLKLLDNWDSVTSTFSK	DYVSQFEGSALGK	a5	b7	45	34	3589.808	1197.61	3	40.46
QLNLKLLDNWDSVTSTFSK	EQLGPVTQEFWDNLEK	a5	b1	45	62	4122.043	1031.519	4	37.9
LLDNWDSVTSTFSKLR	AELQEGAR	a14	b2	59	125	2735.395	684.857	4	29.79
LLDNWDSVTSTFSKLR	AKPALEDLR	a14	b6	59	212	2874.527	575.913	5	22.6
LREQLGPTQEFWDNLEK	VKDLATVYVDVLK	a17	b2	76	12	3644.946	912.244	4	29.42
AKVQPYLDDFQKK	THLAPYSDELRL	a2	b9	96	169	2861.474	573.303	5	51.3
AKVQPYLDDFQKK	THLAPYSDELRL	a2	b8	96	168	2861.465	573.301	5	49.63
AKVQPYLDDFQK	AELQEGAR	a2	b2	96	125	2305.17	577.3	4	45.08
AKVQPYLDDFQKK	DLEEVK	a2	b3	96	91	2292.201	574.058	4	41.05
AKVQPYLDDFQK	VSFLSALEEYTK	a2	b8	96	234	2818.44	705.618	4	37.7
AKVQPYLDDFQKK	LSPLGEEMRDR	a2	b6	96	146	2862.476	573.503	5	31.99
AKVQPYLDDFQK	VSFLSALEEYTK	a2	b9	96	235	2818.443	705.619	4	30.07
VQPYLDDFQK	QKVEPLR	a7	b2	103	118	2102.115	526.537	4	20.88
VQPYLDDFQKK	DLEEVK	a10	b4	106	92	2093.069	524.275	4	27.98
KWQEEMELYL	QKLHELQEK	a4	b2	110	133	2544.255	637.071	4	23.69
KWQEEMELYL	QKLHELQEK	a4	b2	110	133	2544.285	509.865	5	23.44
QKVEPLR	ETEGLR	a2	b1	118	78	1553.854	518.959	3	23.95
QKLHELQEK	AELQEGAR	a2	b2	133	125	2006.058	402.219	5	36.55
LHELQEKLSPLGEEMR	AELQEGAR	a7	b2	140	125	2762.403	921.809	3	43.44
LSPLGEEMR	QKVEPLR	a6	b2	146	118	1881.024	471.264	4	22.15
LSPLGEEMR	QKVEPLR	a7	b2	147	118	1881.015	471.262	4	27.32
LEALKENGGAR	LAEYHAK	a5	b3	182	191	1969.04	493.268	4	33.6

Cross-linking and MS/MS reveals multiple registries in APOA1

LAELYHAKATEHLSTLSEK	LREQLGPVTQEFWDN LEK	a7	b11	195	70	4210.135	843.035	5	36.93
LAELYHAKATEHLSTLSEK	ETEGLR	a7	b3	195	80	2712.372	453.07	6	33.18
LAELYHAKATEHLSTLSEK	DLEEVK	a7	b4	195	92	2740.41	549.09	5	22.12
ATEHLSTLSEK	AKPALEDLR	a3	b2	198	208	2208.176	737.066	3	36.58
ATEHLSTLSEK	AKPALEDLR	a10	b2	205	208	2208.173	737.065	3	32.64
AKPALEDLR	ETEGLR	a2	b1	208	78	1696.911	566.645	3	33.16
AKPALEDLR	AKPALEDLR	a2	b7	208	213	2005.142	402.036	5	32.29
AKPALEDLR	QKLHELQEK	a7	b2	213	133	2145.199	430.048	5	24.39
VSFLSALEEYTK	LEALKENGGAR	a8	b5	234	182	2524.325	842.45	3	38.25
VSFLSALEEYTK	AKPALEDLR	a8	b2	234	208	2379.269	595.825	4	34.51
VSFLSALEEYTKK	VSFLSALEEYTK	a12	b8	238	234	2881.512	721.386	4	22.25
Replicate 2									
Peptide a	Peptide b	CL site a	CL site b	APOA1 Pos1	APOA1 Pos2	Mr	Mz	z	Id- Score
DLATVYVDVLKDSGR	DYVSQFEGSALGK	a11	b1	23	28	3031.508	1011.514	3	26.78
DYVSQFEGSALGKQLNLK	LLDNWDSVTSTFSK	a13	b3	40	48	3589.792	898.456	4	26.9
QLNLKLLDNWDSVTSTFSK	DYVSQFEGSALGK	a5	b7	45	34	3589.803	1197.609	3	48.64
LLDNWDSVTSTFSKLR	AELQEGAR	a14	b2	59	125	2735.391	912.805	3	30.22
LLDNWDSVTSTFSKLR	AELQEGAR	a14	b5	59	128	2735.401	912.808	3	21.69
LLDNWDSVTSTFSKLR	AKPALEDLR	a14	b7	59	213	2874.526	575.913	5	25.57
AELQEGAR	DLEEVKAK	a2	b6	94	125	1784.93	595.984	3	37.77
DYVSQFEGSALGK	AKVQPYLDDFQK	a1	b2	96	28	2832.405	945.143	3	31
AKVQPYLDDFQKK	DLEEVK	a2	b3	96	91	2292.198	459.447	5	40.54
AKVQPYLDDFQK	LSPLGEEMR	a2	b7	96	147	2463.247	616.82	4	23.53
AKVQPYLDDFQKK	THLAPYSDELRL	a2	b8	96	168	2861.476	477.92	6	41.55
AKVQPYLDDFQK	THLAPYSDELRL	a2	b9	96	169	2733.374	684.351	4	41.53

Cross-linking and MS/MS reveals multiple registries in APOA1

AKVQPYLDDFQK	ATEHLSTLSEK	a2	b3	96	198	2647.349	662.845	4	31.48
AKVQPYLDDFQK	ATEHLSTLSEK	a2	b10	96	205	2647.354	662.846	4	32.65
AKVQPYLDDFQK	VSFLSALEEYTK	a2	b8	96	234	2818.446	940.49	3	36.3
VQPYLDDFQKK	DLEEVK	a10	b4	106	92	2093.075	524.276	4	28.21
VQPYLDDFQK	QKVEPLR	a6	b2	118	102	2102.121	526.538	4	20.88
EQLGPVTQEFWDNLEK	QKVEPLR	a9	b2	118	70	2782.429	928.484	3	24.9
LSPLGEEMR	QKVEPLR	a7	b2	118	147	1881.017	628.013	3	28.27
QKLHELQEK	WQEEMELR	a2	b6	133	113	2416.169	605.05	4	20.41
QKLHELQEKLSPLGEEMR	AELQEGAR	a9	b2	140	125	3018.564	604.721	5	42.25
VSFLSALEEYTK	LEALKENGGAR	a8	b5	182	234	2524.335	842.453	3	39.14
LEALKENGGAR	LAEYHAK	a5	b3	182	191	1969.039	657.354	3	33.62
LAEYHAKATEHLSTLSEK	DYVSQFEGSALGK	a7	b1	195	28	3408.692	853.181	4	29.8
LAEYHAKATEHLSTLSEK	LREQLGPVTQEFWDN LEK	a7	b11	195	70	4210.159	1053.548	4	32.58
LAEYHAKATEHLSTLSEK	DLEEVK	a7	b4	195	92	2740.397	549.087	5	24.11
ATEHLSTLSEKAKPALEDLR	THLAPYSDELRL	a11	b8	206	168	3490.814	873.711	4	25.62
ATEHLSTLSEK	AKPALEDLR	a3	b2	208	198	2208.178	442.643	5	34.46
QGLLPVLESFK	AKPALEDLR	a8	b2	208	223	2223.263	556.824	4	29.68
VSFLSALEEYTK	AKPALEDLR	a8	b2	208	234	2379.272	595.826	4	38.02
LREQLGPVTQEFWDNLEK	AKPALEDLR	a11	b2	208	70	3194.678	799.677	4	30.28
ATEHLSTLSEKAKPALEDLR	EQLGPVTQEFWDNLE K	a13	b9	208	70	4122.086	1031.529	4	24.13
AKPALEDLR	ETEGLR	a2	b1	208	78	1696.913	425.236	4	40.04
AKPALEDLR	AKPALEDLR	a2	b6	208	212	2005.137	502.292	4	38.53

Cross-linking and MS/MS reveals multiple registries in APOA1

VSFLSALEEYTKK	ATEHLSTLSEK	a12	b3	238	198	2710.413	543.09	5	25.66
VSFLSALEEYTKK	VSFLSALEEYTK	a12	b8	238	234	2881.51	961.511	3	34.96

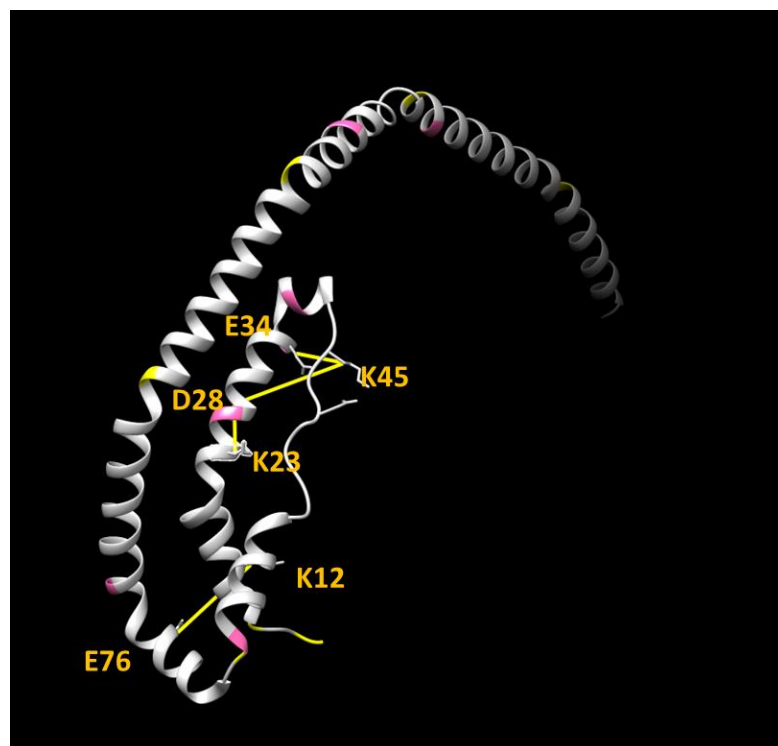
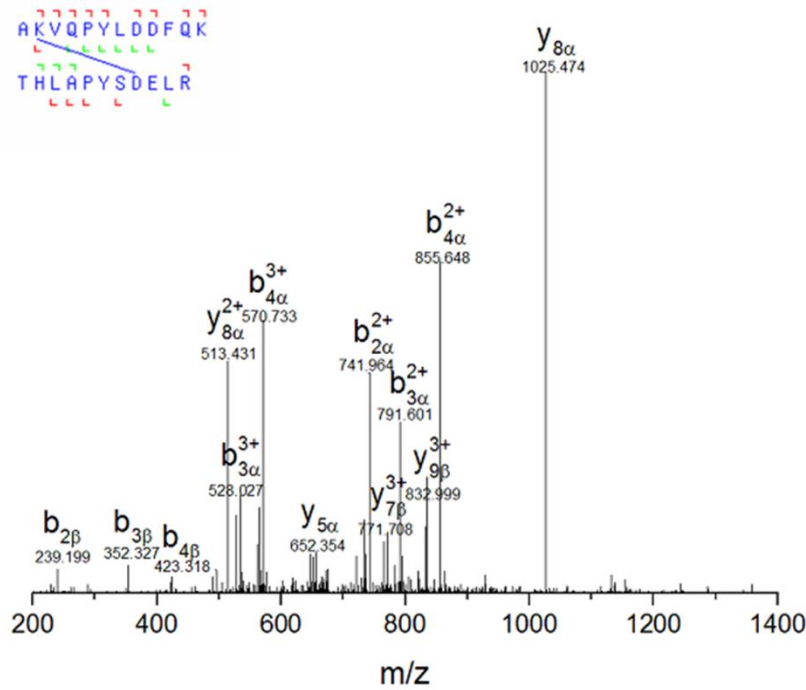


Figure S1. N-terminal cross-links (rHDL) on the crystal structure of N-terminal truncated APOA1 (PDB ID: 3R2P).



Figure S2. Distances of C-terminal cross-links detected in rHDL based on the crystal structure of N-terminal truncated APOA1 (PDB ID:1AV1).

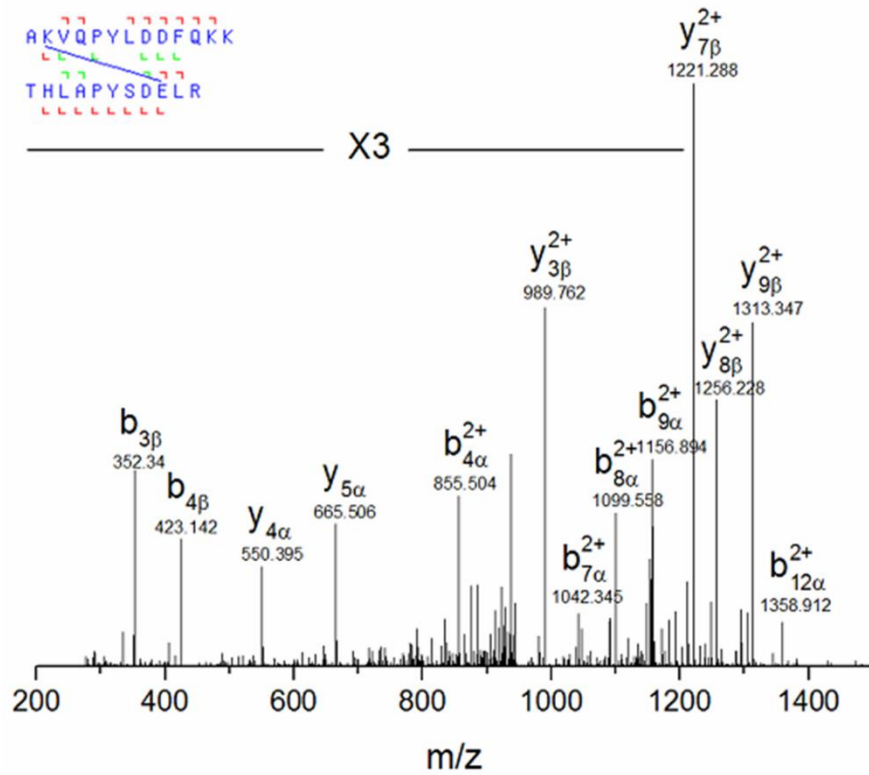
Cross-linking and MS/MS reveals multiple registries in APOA1



K96-D168, m/z: 684.351, Charge state: 4				
fragment type	position	ion th	peak	delta mz
alpha_common_y_standard_plus1	4	537.267	537.342	-0.074
alpha_common_y_standard_plus1	5	652.294	652.354	-0.06
alpha_common_y_standard_plus1	6	765.378	765.442	-0.063
alpha_common_y_standard_plus1	7	928.442	928.413	0.029
alpha_common_y_standard_plus1	8	1025.494	1025.474	0.02
alpha_common_y_standard_plus1	9	1153.553	1153.538	0.015
alpha_common_y_standard_plus2	8	513.251	513.431	-0.18
alpha_xlink_b_standard_plus2	12	1358.691	1358.858	-0.167
alpha_xlink_b_standard_plus2	2	741.889	741.964,742.625	-0.074,-0.736
alpha_xlink_b_standard_plus2	3	791.423	791.601	-0.177
alpha_xlink_b_standard_plus2	4	855.453	855.648	-0.195
alpha_xlink_b_standard_plus3	11	863.431	863.618	-0.186
alpha_xlink_b_standard_plus3	2	494.929	494.949	-0.02
alpha_xlink_b_standard_plus3	3	527.952	528.027	-0.075
alpha_xlink_b_standard_plus3	4	570.638	570.733	-0.096
alpha_xlink_b_standard_plus3	5	602.989	602.979	0.01
alpha_xlink_b_standard_plus3	6	657.343	657.498	-0.155
alpha_xlink_b_standard_plus3	8	733.38	733.422	-0.041
alpha_xlink_b_standard_plus3	9	771.722	771.708	0.015
alpha_xlink_b_standard_plus4	11	647.826	647.609,648.369	0.217,-0.543
alpha_xlink_y_standard_plus4	11	666.593	666.911	-0.318
beta_common_b_standard_plus1	2	239.114	239.199	-0.085
beta_common_b_standard_plus1	3	352.198	352.327	-0.129
beta_common_b_standard_plus1	4	423.236	423.318	-0.083
beta_common_y_standard_plus1	2	288.204	288.289	-0.086
beta_xlink_b_standard_plus2	11	1358.691	1358.858	-0.167
beta_xlink_y_standard_plus2	5	1026.524	1026.606	-0.082
beta_xlink_y_standard_plus3	7	771.391	771.708	-0.317
beta_xlink_y_standard_plus3	8	795.07	795.211	-0.141
beta_xlink_y_standard_plus3	9	832.764	832.999	-0.234

Figure S3.1. The MS/MS spectrum and the list of fragment ions of cross-linked peptide AKVQPYLDDFQK-THLAPYSDEL R in rHDL

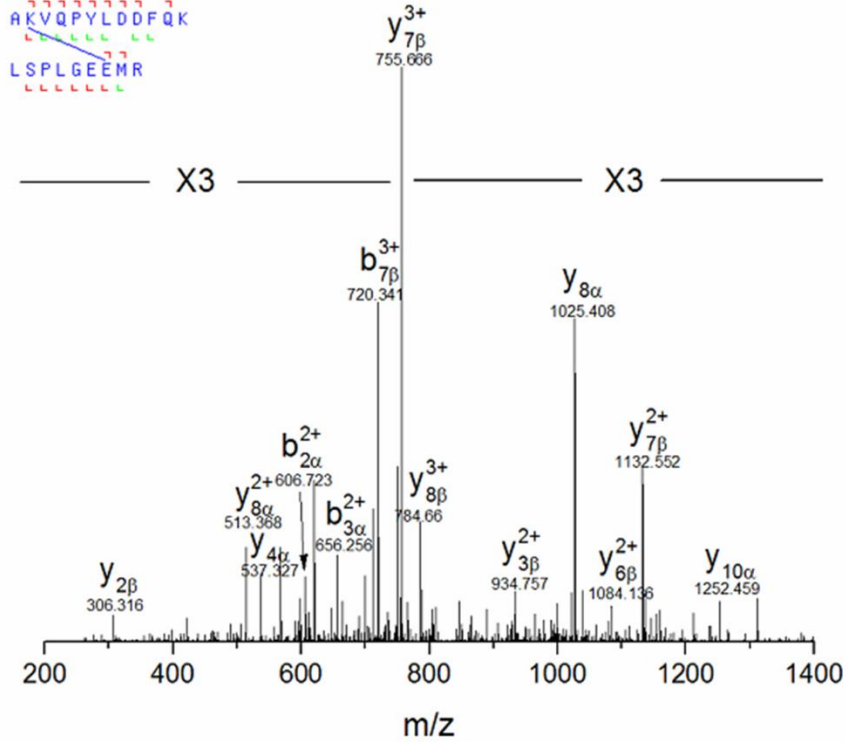
Cross-linking and MS/MS reveals multiple registries in APOA1



K96-E169, m/z: 954.831, Charge state: 3				
fragment type	position	ion th	peak	delta mz
alpha_common_y_standard_plus1	11	1380.716	1380.579	0.137
alpha_common_y_standard_plus1	4	550.335	550.395	-0.059
alpha_common_y_standard_plus1	5	665.362	665.506	-0.144
alpha_common_y_standard_plus1	6	780.389	780.534	-0.144
alpha_common_y_standard_plus1	9	1153.589	1153.545	0.045
alpha_xlink_b_standard_plus2	10	1230.614	1230.995	-0.381
alpha_xlink_b_standard_plus2	11	1294.643	1294.851	-0.208
alpha_xlink_b_standard_plus2	12	1358.691	1358.912	-0.222
alpha_xlink_b_standard_plus2	3	791.423	791.492,792.161	-0.068,-0.737
alpha_xlink_b_standard_plus2	4	855.453	855.504,856.162	-0.051,-0.709
alpha_xlink_b_standard_plus2	7	1042.053	1042.345	-0.293
alpha_xlink_b_standard_plus2	8	1099.566	1099.558,1100.246	0.008,-0.679
alpha_xlink_b_standard_plus2	9	1157.08	1156.894,1157.594	0.185,-0.515
alpha_xlink_b_standard_plus3	11	863.431	863.521	-0.09
alpha_xlink_b_standard_plus3	12	906.13	906.476	-0.346
alpha_xlink_b_standard_plus3	8	733.38	733.805	-0.425
alpha_xlink_y_standard_plus3	12	931.153	931.517	-0.365
beta_common_b_standard_plus1	3	352.198	352.34	-0.142
beta_common_b_standard_plus1	4	423.236	423.142	0.093
beta_common_b_standard_plus1	8	885.411	885.46	-0.049
beta_xlink_b_standard_plus2	10	1344.688	1344.782	-0.095
beta_xlink_b_standard_plus2	9	1288.146	1288.661	-0.515
beta_xlink_y_standard_plus2	3	989.542	989.762	-0.22
beta_xlink_y_standard_plus2	4	1047.055	1047.314	-0.258
beta_xlink_y_standard_plus2	5	1090.571	1090.544,1091.299	0.027,-0.728
beta_xlink_y_standard_plus2	6	1172.103	1172.381	-0.278
beta_xlink_y_standard_plus2	7	1220.63	1220.608,1221.288	0.022,-0.659
beta_xlink_y_standard_plus2	8	1256.148	1256.228,1256.921	-0.079,-0.773
beta_xlink_y_standard_plus2	9	1312.69	1312.693,1313.347	-0.003,-0.657
beta_xlink_y_standard_plus3	10	921.149	921.411	-0.262
beta_xlink_y_standard_plus3	7	814.089	814.179	-0.09
beta_xlink_y_standard_plus3	8	837.768	837.957	-0.189
beta_xlink_y_standard_plus3	9	875.463	875.675	-0.213

Figure S3.2. The MS/MS spectrum and the list of fragment ions of cross-linked peptide AKVQPYLDDFQK-THLAPYSDELRL in rHDL

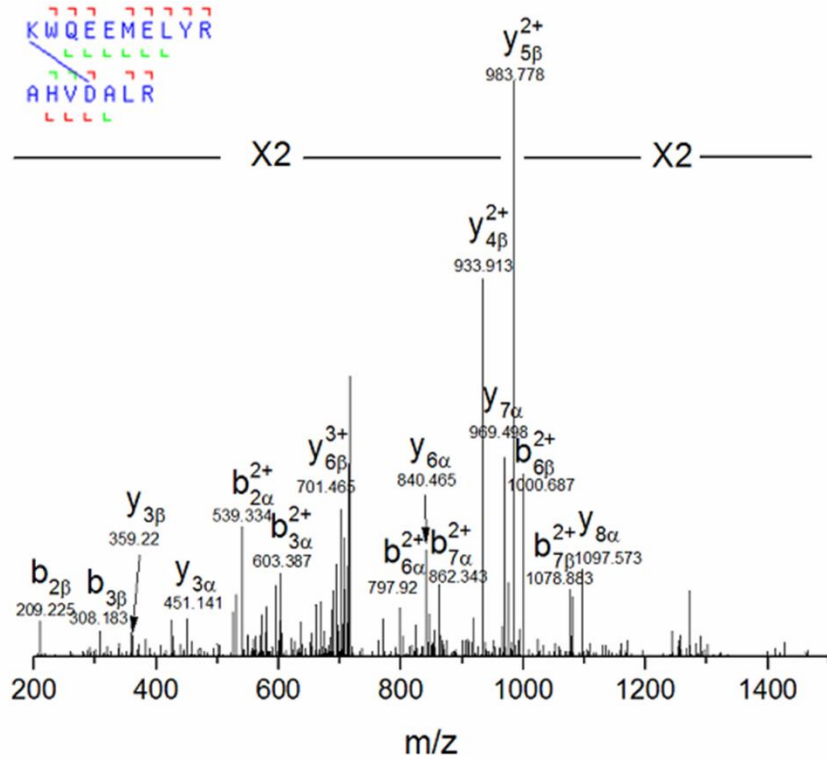
Cross-linking and MS/MS reveals multiple registries in APOA1



K96-E147, m/z: 822.092, Charge state:3				
fragment type	position	ion th	peak	delta mz
alpha_common_y_standard_plus1	10	1252.621	1252.459	0.163
alpha_common_y_standard_plus1	3	422.24	422.24	0
alpha_common_y_standard_plus1	4	537.267	537.327	-0.06
alpha_common_y_standard_plus1	6	765.378	765.253	0.125
alpha_common_y_standard_plus1	7	928.442	928.488	-0.046
alpha_common_y_standard_plus1	8	1025.494	1025.408	0.086
alpha_common_y_standard_plus1	9	1153.553	1153.513	0.04
alpha_common_y_standard_plus2	8	513.251	513.368	-0.117
alpha_xlink_b_standard_plus2	11	1159.578	1159.774	-0.196
alpha_xlink_b_standard_plus2	2	606.824	606.723,607.373	0.101,-0.549
alpha_xlink_b_standard_plus2	3	656.359	656.256	0.103
alpha_xlink_b_standard_plus2	4	720.388	720.341,721.032	0.047,-0.644
alpha_xlink_b_standard_plus2	5	768.914	769.305	-0.391
alpha_xlink_b_standard_plus2	6	850.446	850.574	-0.128
alpha_xlink_b_standard_plus2	7	906.988	906.736	0.252
alpha_xlink_b_standard_plus2	8	964.501	964.421	0.081
alpha_xlink_b_standard_plus2	9	1022.015	1022.113	-0.098
alpha_xlink_b_standard_plus3	5	512.945	513.368	-0.422
alpha_xlink_y_standard_plus3	11	798.411	798.937	-0.526
beta_common_y_standard_plus1	2	306.16	306.316	-0.156
beta_xlink_b_standard_plus2	7	1080.055	1080.184	-0.129
beta_xlink_b_standard_plus2	8	1145.575	1145.649	-0.073
beta_xlink_b_standard_plus3	7	720.373	720.341	0.032
beta_xlink_y_standard_plus2	3	934.473	934.757	-0.284
beta_xlink_y_standard_plus2	4	998.994	999.181	-0.187
beta_xlink_y_standard_plus2	5	1027.505	1027.709	-0.205
beta_xlink_y_standard_plus2	6	1084.047	1084.136,1084.766	-0.089,-0.719
beta_xlink_y_standard_plus2	7	1132.573	1132.552,1133.177	0.021,-0.604
beta_xlink_y_standard_plus3	7	755.385	755.666	-0.281
beta_xlink_y_standard_plus3	8	784.395	784.66	-0.264

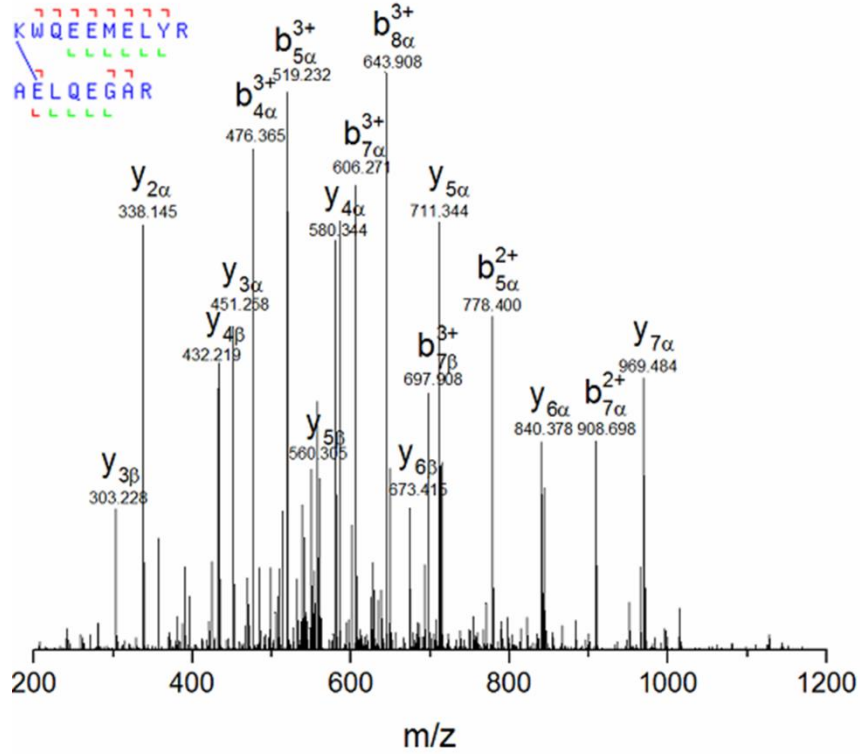
Figure S3.3. The MS/MS spectrum and the list of fragment ions of cross-linked peptide AKVQPYLDDFQK-LSPLGEEMR in rHDL

Cross-linking and MS/MS reveals multiple registries in APOA1



K107-D157, m/z: 725.367, Charge state: 3				
fragment type	position	ion th	peak	delta mz
alpha_common_y_standard_plus1	3	451.267	451.141	0.126
alpha_common_y_standard_plus1	4	580.309	580.25	0.06
alpha_common_y_standard_plus1	5	711.35	711.308	0.042
alpha_common_y_standard_plus1	6	840.393	840.465	-0.072
alpha_common_y_standard_plus1	7	969.435	969.498	-0.063
alpha_common_y_standard_plus1	8	1097.494	1097.573	-0.079
alpha_xlink_b_standard_plus2	10	1078.539	1078.883	-0.344
alpha_xlink_b_standard_plus2	2	539.302	539.334	-0.032
alpha_xlink_b_standard_plus2	3	603.331	603.387	-0.056
alpha_xlink_b_standard_plus2	4	667.852	667.952	-0.1
alpha_xlink_b_standard_plus2	6	797.894	797.92	-0.026
alpha_xlink_b_standard_plus2	7	862.415	862.343,863.084	0.072,-0.669
alpha_xlink_b_standard_plus2	8	918.957	919.045	-0.088
alpha_xlink_b_standard_plus2	9	1000.489	1000.687	-0.198
alpha_xlink_b_standard_plus3	9	667.329	667.952	-0.624
beta_common_b_standard_plus1	2	209.104	209.225	-0.121
beta_common_b_standard_plus1	3	308.172	308.183	-0.011
beta_common_y_standard_plus1	3	359.241	359.22	0.021
beta_xlink_b_standard_plus2	4	908.428	908.718	-0.29
beta_xlink_b_standard_plus2	6	1000.489	1000.687	-0.198
beta_xlink_b_standard_plus2	7	1078.539	1078.883	-0.344
beta_xlink_b_standard_plus3	6	667.329	667.952	-0.624
beta_xlink_y_standard_plus2	4	933.963	933.913,934.648	0.049,-0.685
beta_xlink_y_standard_plus2	5	983.497	983.778	-0.282
beta_xlink_y_standard_plus3	6	701.687	701.465,702.102	0.222,-0.415

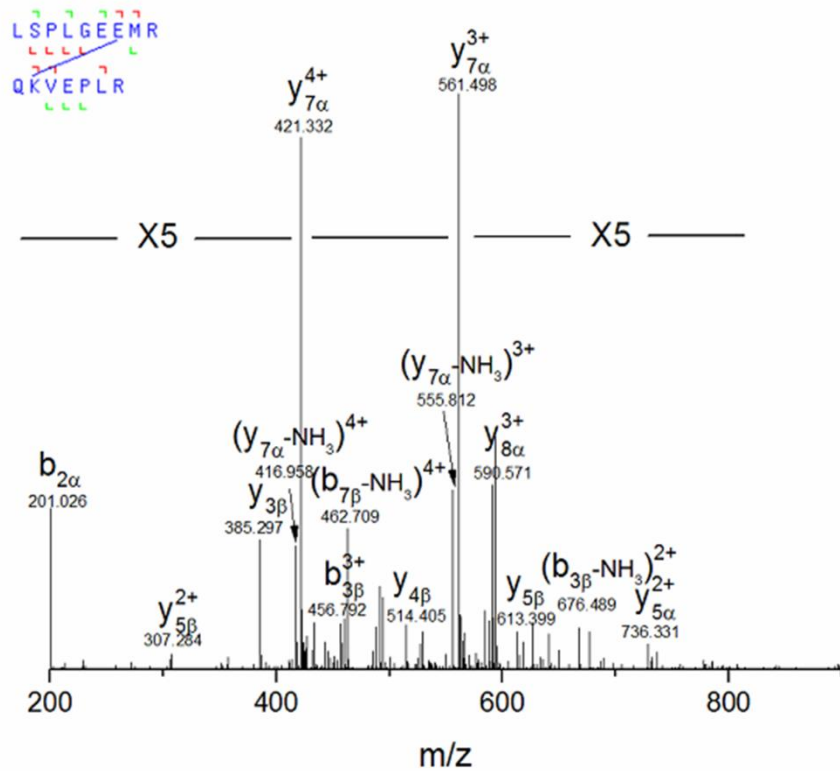
Figure S3.4. The MS/MS spectrum and the list of fragment ions of cross-linked peptide **KWQEEMELYR-AHVDALR** in rHDL



K107-E125, m/z: 567.279, Charge state: 4

fragment type	position	ion th	peak	delta mz
alpha common y standard plus1	2	338.183	338.145	0.038
alpha common y standard plus1	3	451.267	451.258	0.009
alpha common y standard plus1	4	580.309	580.344	-0.035
alpha common y standard plus1	5	711.35	711.344	0.006
alpha common y standard plus1	6	840.393	840.378	0.015
alpha common y standard plus1	7	969.435	969.484	-0.049
alpha common y standard plus2	7	485.221	485.142	0.08
alpha xlink b standard plus2	2	585.307	585.380,586.016	-0.073,-0.709
alpha xlink b standard plus2	3	649.337	649.313,650.097	0.024,-0.760
alpha xlink b standard plus2	4	713.858	713.738,714.576	0.120,-0.718
alpha xlink b standard plus2	5	778.379	778.400,779.103	-0.021,-0.724
alpha xlink b standard plus2	6	843.899	844.104	-0.205
alpha xlink b standard plus2	7	908.421	908.698	-0.277
alpha xlink b standard plus2	8	964.963	965.309	-0.346
alpha xlink b standard plus3	2	390.541	390.66	-0.119
alpha xlink b standard plus3	3	433.227	433.388	-0.161
alpha xlink b standard plus3	4	476.241	476.365	-0.124
alpha xlink b standard plus3	5	519.255	519.232,519.865	0.024,-0.610
alpha xlink b standard plus3	7	605.95	606.271	-0.321
alpha xlink b standard plus3	8	643.644	643.908	-0.263
alpha xlink b standard plus3	9	697.999	697.908,698.622	0.091,-0.623
beta common y standard plus1	3	303.178	303.228	-0.05
beta common y standard plus1	4	432.221	432.219	0.001
beta common y standard plus1	5	560.279	560.305	-0.026
beta common y standard plus1	6	673.363	673.415	-0.051
beta common y standard plus2	6	337.186	337.3	-0.114
beta xlink b standard plus2	2	797.372	797.593	-0.221
beta xlink b standard plus3	2	531.918	531.941	-0.024
beta xlink b standard plus3	6	674.32	674.387	-0.067
beta xlink b standard plus3	7	697.999	697.908,698.622	0.091,-0.623
beta xlink y standard plus4	7	549.52	549.528	-0.008

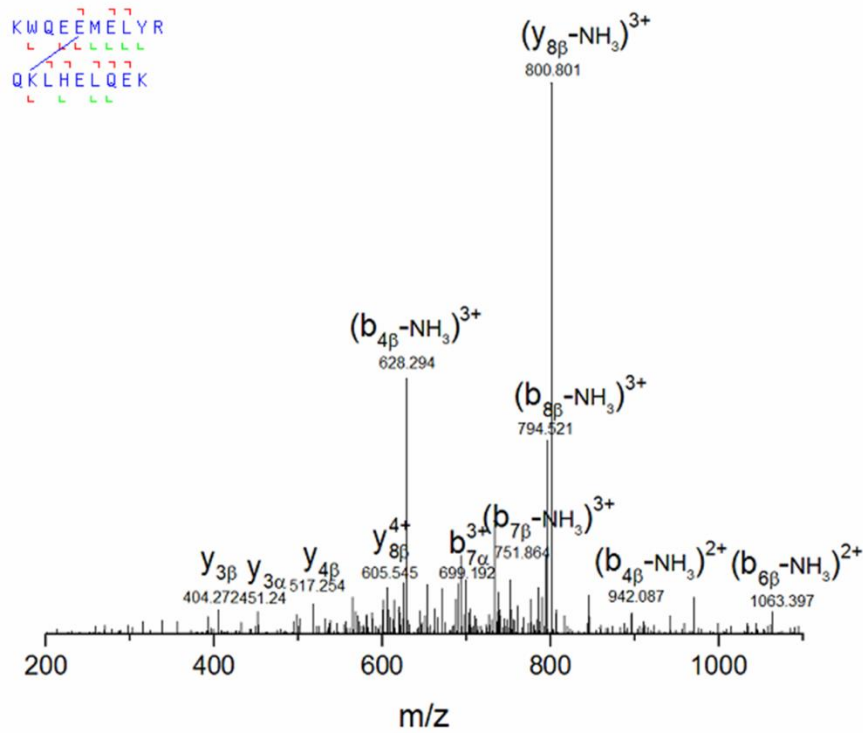
Figure S3.5. The MS/MS spectrum and the list of fragment ions of cross-linked peptide **KWQEEMELYR-AELQEGAR** in rHDL



K118-E147, m/z: 471.262, Charge state: 4

fragment type	position	ion th	peak	delta mz
alpha_common_b_standard_plus1	2	201.124	201.026	0.098
alpha_common_b_standard_plus1	4	411.261	411.192	0.069
alpha_common_b_standard_plus1	6	597.325	597.238	0.086
alpha_common_y_standard_plus1	2	306.16	306.329	-0.169
alpha_xlink_b_standard_plus3	7	526.295	526.923	-0.627
alpha_xlink_b_standard_plus3	8	569.975	569.834	0.141
alpha_xlink_b_standard_plus4	8	427.733	427.458	0.275
alpha_xlink_y_-NH3_plus3	7	555.632	555.812	-0.181
alpha_xlink_y_-NH3_plus4	7	416.976	416.958	0.018
alpha_xlink_y_standard_plus2	5	736.388	736.331	0.058
alpha_xlink_y_standard_plus3	5	491.262	491.499	-0.237
alpha_xlink_y_standard_plus3	6	528.956	529.186	-0.229
alpha_xlink_y_standard_plus3	7	561.307	561.498	-0.191
alpha_xlink_y_standard_plus3	8	590.318	590.571	-0.253
alpha_xlink_y_standard_plus4	7	421.232	421.332	-0.099
alpha_xlink_y_standard_plus4	8	442.99	443.053	-0.063
beta_common_y_standard_plus1	3	385.256	385.297	-0.041
beta_common_y_standard_plus1	4	514.299	514.405	-0.107
beta_common_y_standard_plus1	5	613.367	613.399	-0.032
beta_common_y_standard_plus2	5	307.188	307.284	-0.097
beta_xlink_b_-NH3_plus2	3	676.356	676.489	0.19
beta_xlink_b_-NH3_plus4	7	462.502	462.709	-0.207
beta_xlink_b_standard_plus2	2	635.335	635.285	0.05
beta_xlink_b_standard_plus3	2	423.893	424.175	-0.282
beta_xlink_b_standard_plus3	3	456.916	456.792	0.124
beta_xlink_b_standard_plus3	6	569.975	569.834	0.141
beta_xlink_b_standard_plus4	6	427.733	427.458	0.275

Figure S3.6. The MS/MS spectrum and the list of fragment ions of cross-linked peptide LSPLGEE MR-QKVEPLR in rHDL

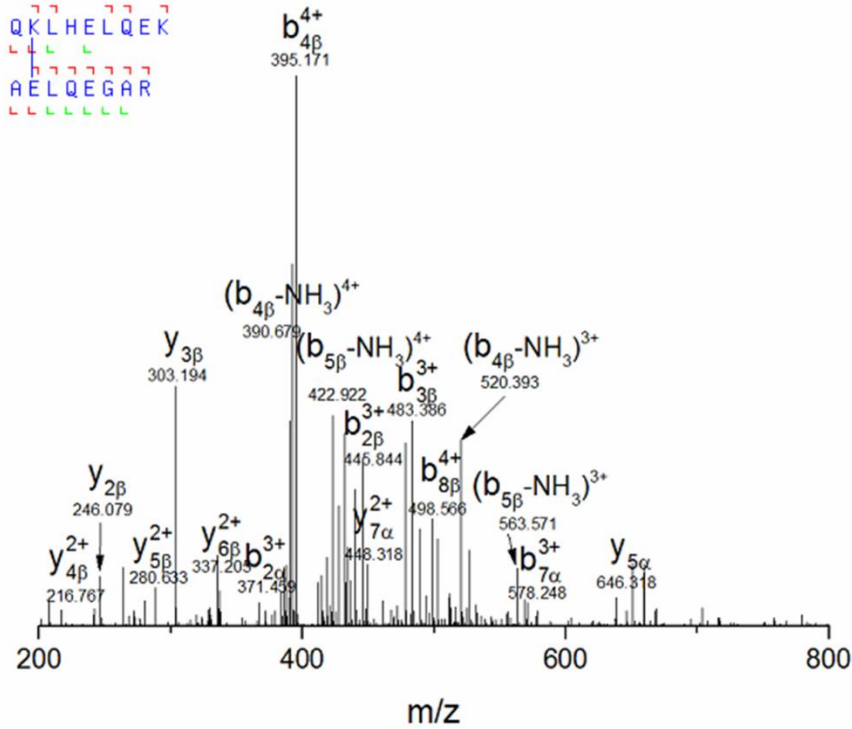


K133-E111, m/z: 637.078, Charge state: 4

fragment type	position	ion th	peak	delta mz
alpha_common_y_standard_plus1	2	338.183	338.244	-0.061
alpha_common_y_standard_plus1	3	451.267	451.24	0.027
alpha_common_y_standard_plus1	4	580.309	580.481	-0.172
alpha_common_y_standard_plus1	5	711.35	711.262	0.088
alpha_common_y_standard_plus2	5	356.179	356.061	0.118
alpha_xlink_b_standard_plus3	5	612.32	612.692	-0.372
alpha_xlink_b_standard_plus3	7	699.015	699.192	-0.178
alpha_xlink_b_standard_plus3	8	736.709	737.068	-0.359
alpha_xlink_y_standard_plus3	7	701.69	702.191	-0.501
alpha_xlink_y_standard_plus3	9	806.403	806.360,807.023	0.043,-0.620
alpha_xlink_y_standard_plus4	6	494.259	494.503	-0.244
alpha_xlink_y_standard_plus4	9	605.054	605.545	-0.491
beta_common_y_standard_plus1	3	404.215	404.272	-0.058
beta_common_y_standard_plus1	4	517.299	517.254	0.045
beta_common_y_standard_plus1	6	783.4	783.537	-0.137
beta_xlink_b_-NH3_plus2	4	941.968	942.087	-0.119
beta_xlink_b_-NH3_plus2	6	1063.031	1063.397	-0.367
beta_xlink_b_-NH3_plus3	4	628.314	628.294	0.02
beta_xlink_b_-NH3_plus3	7	751.709	751.864	-0.155
beta_xlink_b_-NH3_plus3	8	794.724	794.521,795.132	0.202,-0.409
beta_xlink_b_standard_plus3	3	588.304	588.54	-0.236
beta_xlink_b_standard_plus3	7	757.385	757.669	-0.284
beta_xlink_b_standard_plus3	8	800.399	800.801	-0.402
beta_xlink_b_standard_plus4	7	568.291	568.352	-0.061
beta_xlink_b_standard_plus4	8	600.551	600.486	0.066
beta_xlink_y_-NH3_plus3	8	800.739	800.801	-0.062
beta_xlink_y_standard_plus3	8	806.415	806.360,807.023	0.055,-0.608
beta_xlink_y_standard_plus4	8	605.063	605.545	-0.482

Figure S3.7. The MS/MS spectrum and the list of fragment ions of cross-linked peptide KWQEEMELYR-QKLHELQEK in rHDL

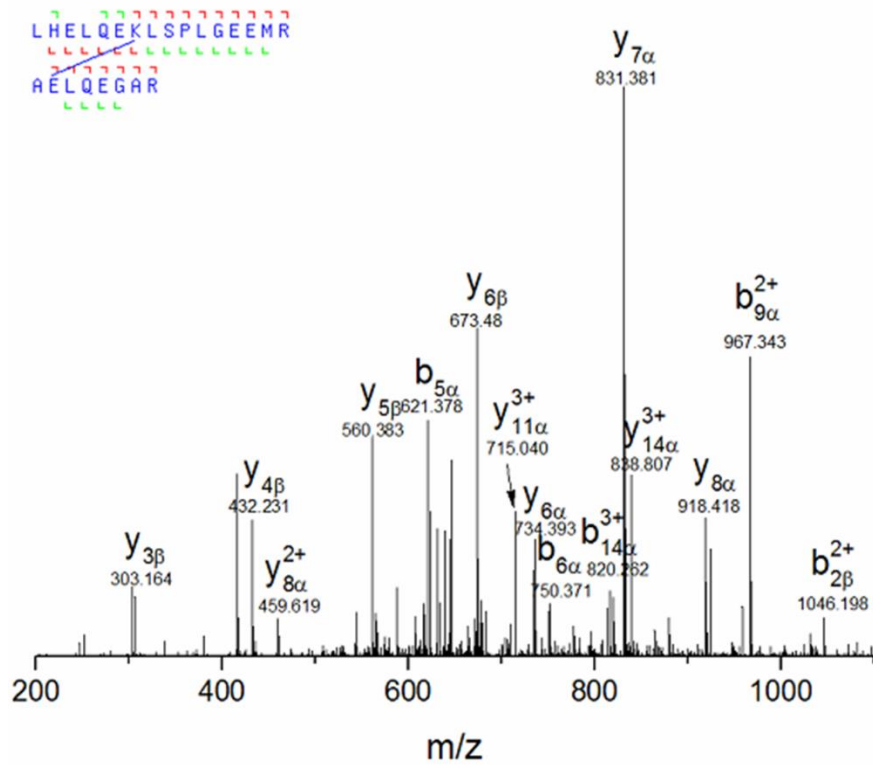
Cross-linking and MS/MS reveals multiple registries in APOA1



K133-E125, m/z: 402.22, Charge state: 5

fragment type	position	ion th	peak	delta mz
alpha_common_y_standard_plus1	5	646.341	646.318	0.023
alpha_common_y_standard_plus2	7	448.746	448.828	-0.082
alpha_xlink_b_standard_plus2	2	556.297	556.772	-0.475
alpha_xlink_b_standard_plus3	2	371.201	371.459	-0.259
alpha_xlink_b_standard_plus3	6	535.29	535.377	-0.087
alpha_xlink_b_standard_plus3	7	577.977	578.248	-0.271
alpha_xlink_b_standard_plus4	9	498.019	498.566	-0.547
alpha_xlink_b_standard_plus5	3	245.74	246.079	-0.339
beta_common_y_standard_plus1	2	246.157	246.079	0.078
beta_common_y_standard_plus1	3	303.178	303.194	-0.016
beta_common_y_standard_plus1	4	432.221	432.239	-0.018
beta_common_y_standard_plus2	4	216.614	216.767	-0.153
beta_common_y_standard_plus2	5	280.644	280.633	0.011
beta_common_y_standard_plus2	6	337.186	337.205	-0.02
beta_xlink_b_-NH3_plus3	4	520.28	520.393	-0.114
beta_xlink_b_-NH3_plus3	5	563.294	563.571	-0.278
beta_xlink_b_-NH3_plus4	4	390.462	390.679	-0.217
beta_xlink_b_-NH3_plus4	5	422.722	422.922	-0.2
beta_xlink_b_-NH3_plus5	8	395.211	395.171	0.041
beta_xlink_b_standard_plus2	2	667.857	667.886	-0.028
beta_xlink_b_standard_plus3	2	445.574	445.844	-0.27
beta_xlink_b_standard_plus3	3	483.269	483.386	-0.117
beta_xlink_b_standard_plus3	4	525.955	526.265	-0.31
beta_xlink_b_standard_plus3	5	568.969	568.946	0.023
beta_xlink_b_standard_plus4	4	394.718	395.171	-0.452
beta_xlink_b_standard_plus4	5	426.979	427.276	-0.297
beta_xlink_b_standard_plus4	6	441.234	440.983,441.677	0.251,-0.443
beta_xlink_b_standard_plus4	8	498.019	498.566	-0.547
beta_xlink_b_standard_plus5	2	267.748	268.07	-0.322
beta_xlink_b_standard_plus5	7	367.396	367.263	0.134
beta_xlink_y_standard_plus3	7	646.014	646.318	-0.304
beta_xlink_y_standard_plus4	8	502.521	502.372	0.149
beta_xlink_y_standard_plus5	7	388.011	387.858	0.153

Figure S3.8. The MS/MS spectrum and the list of fragment ions of cross-linked peptide QKLHELQEK-AELQEGAR in rHDL

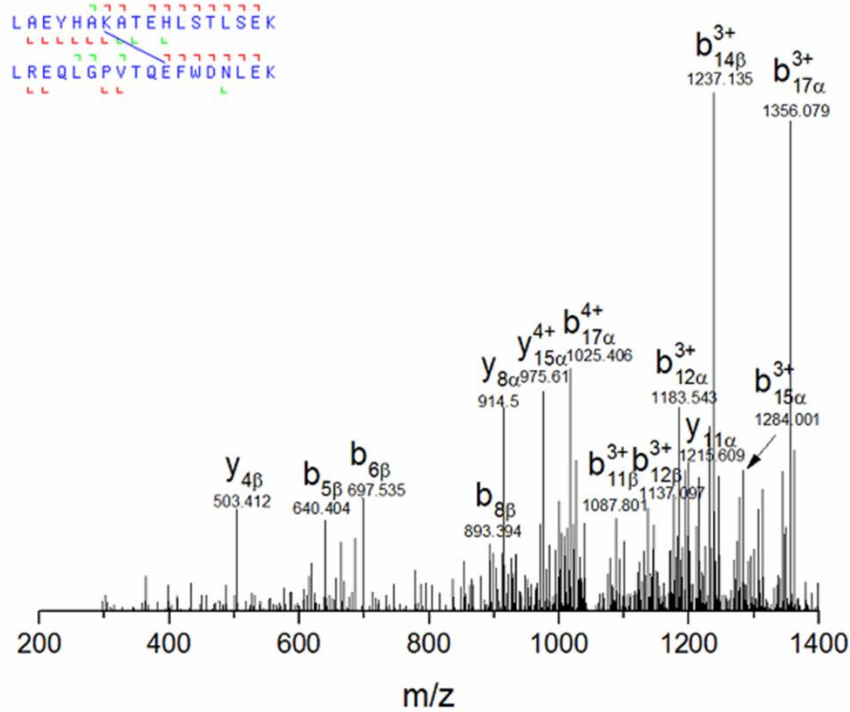


K140-E125, m/z: 691.609, Charge state: 4

fragment type	position	ion th	peak	delta mz
alpha_common_b_standard_plus1	2	251.151	251.14	0.011
alpha_common_b_standard_plus1	5	621.336	621.378	-0.041
alpha_common_b_standard_plus1	8	750.379	750.371	0.008
alpha_common_y_standard_plus1	2	306.16	306.143	0.017
alpha_common_y_standard_plus1	3	435.203	435.276	-0.073
alpha_common_y_standard_plus1	4	564.245	564.42	-0.175
alpha_common_y_standard_plus1	5	621.267	621.378	-0.111
alpha_common_y_standard_plus1	6	734.351	734.393	-0.042
alpha_common_y_standard_plus1	7	831.403	831.381	0.023
alpha_common_y_standard_plus1	8	918.435	918.418	0.018
alpha_common_y_standard_plus1	9	1031.52	1031.553	-0.033
alpha_common_y_standard_plus2	8	459.722	459.619	0.102
alpha_xlink_b_standard_plus2	16	1373.2	1373.889	-0.686
alpha_xlink_b_standard_plus2	7	866.953	867.409	-0.456
alpha_xlink_b_standard_plus2	8	923.495	923.927	-0.432
alpha_xlink_b_standard_plus2	9	967.011	967.343	-0.332
alpha_xlink_b_standard_plus3	10	677.361	677.376	-0.015
alpha_xlink_b_standard_plus3	11	715.056	715.040,715.646	0.016,-0.591
alpha_xlink_b_standard_plus3	12	734.063	734.393	-0.33
alpha_xlink_b_standard_plus3	13	777.077	777.313	-0.236
alpha_xlink_b_standard_plus3	14	820.091	820.262	-0.171
alpha_xlink_b_standard_plus3	15	863.771	864.031	-0.26
alpha_xlink_b_standard_plus3	8	615.999	616.227	-0.228
alpha_xlink_b_standard_plus3	9	645.01	645.059	-0.049
alpha_xlink_y_standard_plus3	10	672.018	671.799	0.219
alpha_xlink_y_standard_plus3	11	715.032	715.040,715.646	-0.007,-0.614
alpha_xlink_y_standard_plus3	12	757.719	758.088	-0.369
alpha_xlink_y_standard_plus3	13	795.413	795.57	-0.157
alpha_xlink_y_standard_plus3	14	838.428	838.807	-0.38
alpha_xlink_y_standard_plus4	15	863.337	863.611	-0.273
beta_common_y_standard_plus1	3	303.178	303.164	0.014
beta_common_y_standard_plus1	4	432.221	432.231	-0.01
beta_common_y_standard_plus1	5	560.279	560.383	-0.104
beta_common_y_standard_plus1	6	673.363	673.48	-0.117
beta_common_y_standard_plus2	6	337.186	337.284	-0.099
beta_xlink_b_standard_plus2	2	1046.03	1046.198	-0.167
beta_xlink_b_standard_plus2	8	1373.2	1373.889	-0.686
beta_xlink_b_standard_plus3	3	735.385	735.656	-0.271
beta_xlink_b_standard_plus3	4	778.071	778.367	-0.296
beta_xlink_b_standard_plus3	5	821.085	821.147	-0.062
beta_xlink_b_standard_plus3	7	863.771	864.031	-0.26
beta_xlink_b_standard_plus4	5	616.066	616.227	-0.161
beta_xlink_b_standard_plus4	6	630.321	630.787	-0.466

Figure S3.9. The MS/MS spectrum and the list of fragment ions of cross-linked peptide LHELQEKLSPLGEE MR-AELQEGAR in rHDL

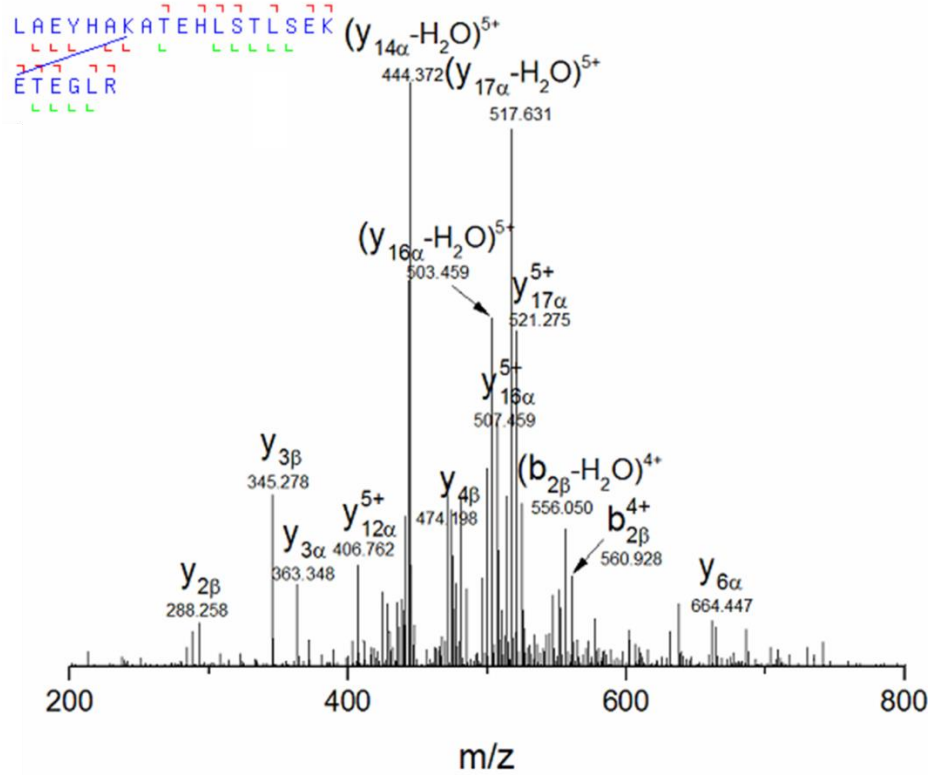
Cross-linking and MS/MS reveals multiple registries in APOA1



195-70, m/z: 1053.543, Charge state: 4

fragment type	position	ion th	peak	delta mz
alpha_common_b_standard_plus1	6	685.331	685.22	0.111
alpha_common_y_standard_plus1	10	1144.585	1144.439	0.146
alpha_common_y_standard_plus1	11	1215.622	1215.609	0.013
alpha_common_y_standard_plus1	8	914.495	914.5	-0.005
alpha_xlink_b_standard_plus3	10	1099.89	1099.925	-0.035
alpha_xlink_b_standard_plus3	11	1145.576	1145.523	0.053
alpha_xlink_b_standard_plus3	12	1183.271	1183.543	-0.272
alpha_xlink_b_standard_plus3	13	1212.282	1212.62	-0.338
alpha_xlink_b_standard_plus3	14	1245.964	1245.737,1246.526	0.227,-0.562
alpha_xlink_b_standard_plus3	15	1283.659	1284.001	-0.342
alpha_xlink_b_standard_plus3	16	1312.67	1312.957	-0.287
alpha_xlink_b_standard_plus3	17	1355.684	1356.079	-0.395
alpha_xlink_b_standard_plus3	7	999.514	999.845	-0.331
alpha_xlink_b_standard_plus3	8	1023.193	1023.142,1023.774	0.051,-0.580
alpha_xlink_b_standard_plus4	17	1017.015	1017.282	-0.267
alpha_xlink_y_standard_plus3	12	1176.278	1176.114	0.164
alpha_xlink_y_standard_plus3	13	1199.957	1200.082	-0.125
alpha_xlink_y_standard_plus3	14	1245.643	1245.737	-0.094
alpha_xlink_y_standard_plus4	15	975.25	975.61	-0.359
alpha_xlink_y_standard_plus4	16	1007.511	1007.585	-0.074
alpha_xlink_y_standard_plus4	17	1025.27	1025.406	-0.136
beta_common_b_standard_plus1	5	640.378	640.404	-0.026
beta_common_b_standard_plus1	6	697.4	697.535	-0.136
beta_common_b_standard_plus1	8	893.521	893.394	0.127
beta_common_y_standard_plus1	4	503.283	503.412	-0.129
beta_xlink_b_standard_plus3	11	1087.569	1087.801	-0.232
beta_xlink_b_standard_plus3	12	1136.592	1137.097	-0.505
beta_xlink_b_standard_plus3	13	1198.618	1198.841	-0.223
beta_xlink_b_standard_plus3	14	1236.961	1237.135	-0.175
beta_xlink_b_standard_plus3	15	1274.975	1275.192	-0.217
beta_xlink_b_standard_plus3	16	1312.67	1312.957	-0.287
beta_xlink_b_standard_plus3	17	1355.684	1356.079	-0.395
beta_xlink_b_standard_plus4	17	1017.015	1017.282	-0.267
beta_xlink_y_standard_plus3	11	1139.904	1140.5	-0.596
beta_xlink_y_standard_plus3	12	1172.255	1172.409	-0.154
beta_xlink_y_standard_plus3	16	1314.657	1314.809	-0.152
beta_xlink_y_standard_plus4	17	1025.27	1025.406	-0.136

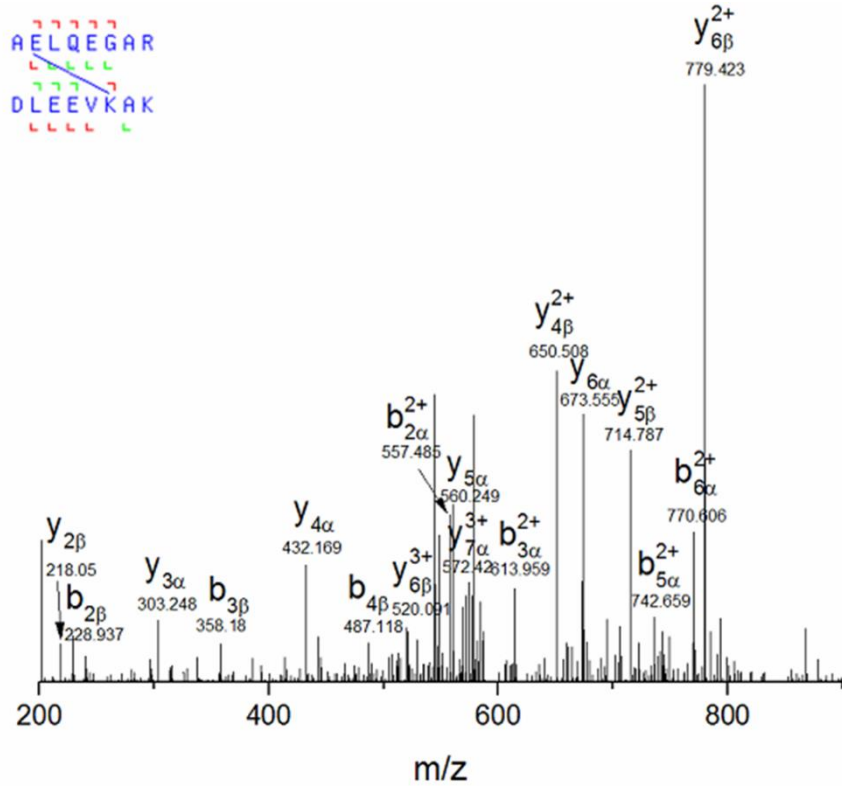
Figure S3.10. The MS/MS spectrum and the list of fragment ions of cross-linked peptide LAEYHAKATEHLSTLSEK-LREQLGPVTQEFWDNLEK in rHDL



K195-E78, m/z: 453.073, Charge state: 6

fragment type	position	ion th	peak	delta mz
alpha_common_y_standard_plus1	3	363.188	363.348	-0.16
alpha_common_y_standard_plus1	4	476.272	476.13	0.142
alpha_common_y_standard_plus1	5	577.32	577.15	0.17
alpha_common_y_standard_plus1	6	664.352	664.447	-0.096
alpha_common_y_standard_plus2	10	572.796	572.684	0.113
alpha_common_y_standard_plus2	7	389.222	389.223	-0.001
alpha_xlink_b_standard_plus4	11	484.994	485.294	-0.3
alpha_xlink_b_standard_plus4	13	535.023	535.397	-0.374
alpha_xlink_b_standard_plus4	15	588.556	588.851	-0.295
alpha_xlink_b_standard_plus4	9	418.468	418.187	0.281
alpha_xlink_b_standard_plus5	12	410.813	411.177	-0.364
alpha_xlink_b_standard_plus5	15	471.046	471.342	-0.296
alpha_xlink_b_standard_plus5	17	514.261	514.068	0.193
alpha_xlink_b_standard_plus5	18	539.88	540.372	-0.492
alpha_xlink_y_-H2O_plus5	14	444.635	444.372	0.263
alpha_xlink_y_-H2O_plus5	16	503.056	503.459	-0.403
alpha_xlink_y_-H2O_plus5	17	517.263	517.631	-0.368
alpha_xlink_y_standard_plus4	12	508.02	508.155	-0.135
alpha_xlink_y_standard_plus4	13	525.779	525.916	-0.136
alpha_xlink_y_standard_plus5	12	406.618	406.762	-0.145
alpha_xlink_y_standard_plus5	15	480.849	480.981	-0.131
alpha_xlink_y_standard_plus5	16	506.658	507.02	-0.362
alpha_xlink_y_standard_plus5	17	520.865	521.275	-0.41
beta_common_y_standard_plus1	2	288.204	288.258	-0.054
beta_common_y_standard_plus1	3	345.225	345.278	-0.053
beta_common_y_standard_plus1	4	474.268	474.198	0.07
beta_common_y_standard_plus2	5	288.162	288.258	-0.096
beta_xlink_b_-H2O_plus4	2	556.283	556.050,556.657	0.233,-0.373
beta_xlink_b_standard_plus4	1	535.524	535.397	0.127
beta_xlink_b_standard_plus4	2	560.786	560.928	-0.142
beta_xlink_b_standard_plus5	1	428.621	428.751	-0.131
beta_xlink_b_standard_plus5	3	474.639	475.059	-0.42
beta_xlink_b_standard_plus5	5	508.66	508.994	-0.334
beta_xlink_b_standard_plus5	6	539.88	540.372	-0.492

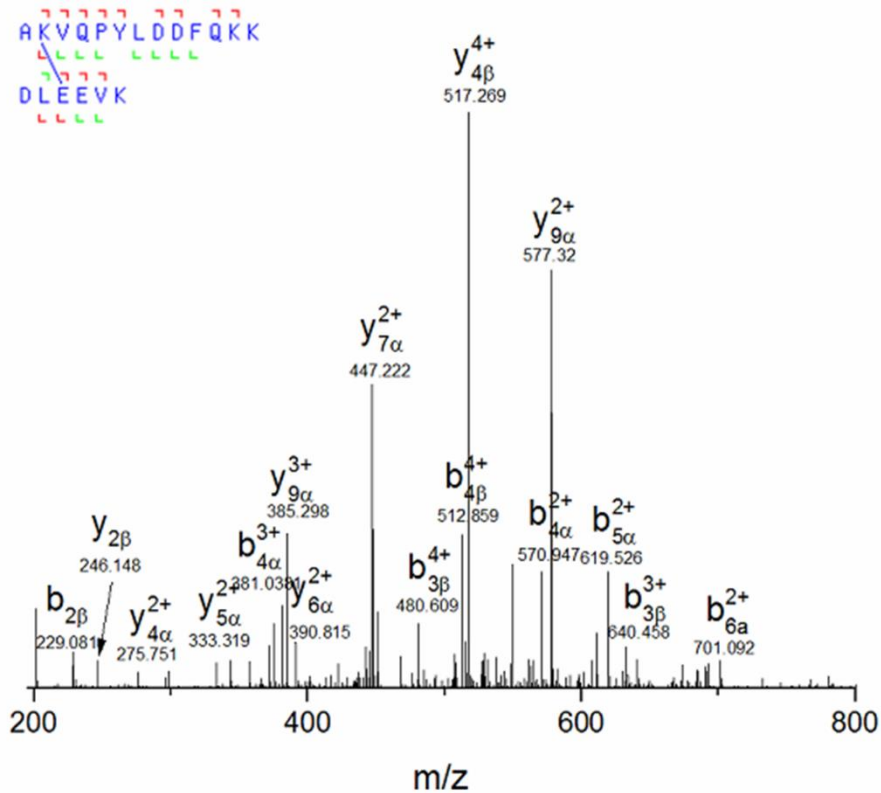
Figure S3.11. The MS/MS spectrum and the list of fragment ions of cross-linked peptide LAEYHAKATEHLSTLSEK-ETEGLR in rHDL



K94-E125, m/z: 595.984, Charge state: 3

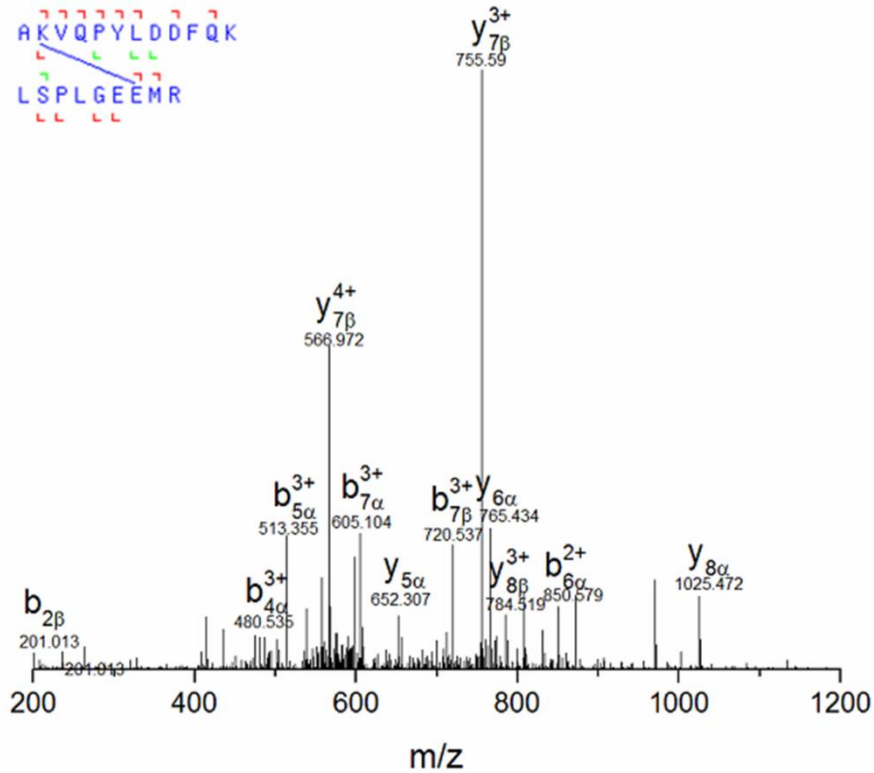
fragment type	position	ion th	peak	delta mz
alpha_common_y_standard_plus1	3	303.178	303.248	-0.07
alpha_common_y_standard_plus1	4	432.221	432.169	0.051
alpha_common_y_standard_plus1	5	560.279	560.249	0.03
alpha_common_y_standard_plus1	6	673.363	673.555	-0.192
alpha_common_y_standard_plus2	6	337.186	337.359	-0.173
alpha_xlink_b_standard_plus2	2	557.294	557.485	-0.191
alpha_xlink_b_standard_plus2	3	613.836	613.959	-0.124
alpha_xlink_b_standard_plus2	4	677.865	677.851	0.014
alpha_xlink_b_standard_plus2	5	742.386	742.659	-0.273
alpha_xlink_b_standard_plus2	6	770.897	770.606,771.373	0.290,-0.476
alpha_xlink_b_standard_plus3	6	514.267	514.336	-0.069
alpha_xlink_y_standard_plus3	7	572.304	572.42	-0.115
beta_common_b_standard_plus1	2	229.119	228.937	0.182
beta_common_b_standard_plus1	3	358.161	358.18	-0.019
beta_common_b_standard_plus1	4	487.204	487.118	0.086
beta_common_y_standard_plus1	2	218.15	218.05	0.1
beta_xlink_b_standard_plus2	6	784.9	784.643	0.257
beta_xlink_y_standard_plus2	4	650.373	650.508	-0.135
beta_xlink_y_standard_plus2	5	714.894	714.787,715.462	0.108,-0.567
beta_xlink_y_standard_plus2	6	779.416	779.423,780.058	-0.007,-0.642
beta_xlink_y_standard_plus3	6	519.946	520.091	-0.145
beta_xlink_y_standard_plus3	7	557.641	557.485	0.156

Figure S4.1. The MS/MS spectrum and the list of fragment ions of cross-linked peptide AELQEGAR-DLEEVKAK in human HDL



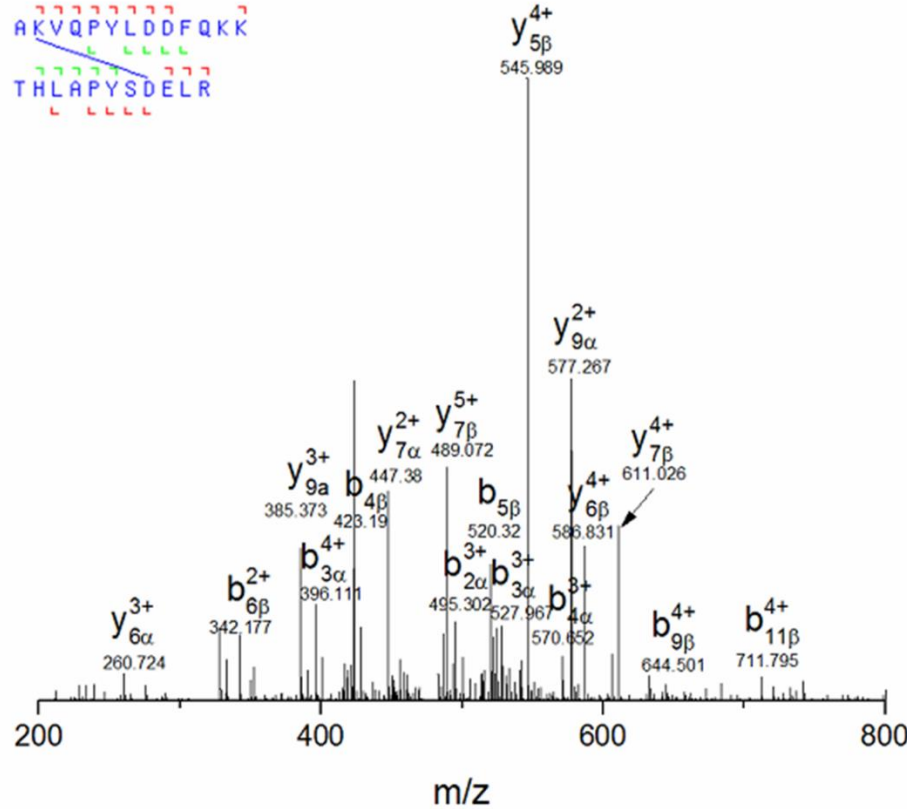
K96-E91, m/z: 459.447, Charge state: 5				
fragment type	position	ion th	peak	delta mz
alpha common y standard plus1	6	780.389	780.379	0.01
alpha common y standard plus2	10	641.328	641.311	0.017
alpha common y standard plus2	11	690.862	690.748	0.114
alpha common y standard plus2	4	275.672	275.751	-0.079
alpha common y standard plus2	5	333.185	333.319	-0.134
alpha common y standard plus2	6	390.699	390.815	-0.117
alpha common y standard plus2	7	447.241	447.222	0.019
alpha common y standard plus2	9	577.299	577.32	-0.022
alpha common y standard plus3	7	298.496	298.506	-0.01
alpha common y standard plus3	9	385.202	385.298	-0.096
alpha xlink b standard plus2	3	506.788	507.025	-0.237
alpha xlink b standard plus2	4	570.817	570.947	-0.13
alpha xlink b standard plus2	5	619.344	619.526	-0.182
alpha xlink b standard plus2	6	700.875	701.092	-0.217
alpha xlink b standard plus3	11	673.674	673.623	0.051
alpha xlink b standard plus3	4	380.881	381.038	-0.157
alpha xlink b standard plus3	6	467.586	467.757	-0.171
alpha xlink b standard plus3	8	543.623	543.803	-0.18
alpha xlink b standard plus3	9	581.965	582.35	-0.385
alpha xlink b standard plus4	12	537.531	537.666	-0.135
alpha xlink b standard plus4	2	229.131	229.081	0.05
alpha xlink b standard plus4	9	436.726	437.083	-0.357
beta common b standard plus1	2	229.119	229.081	0.038
beta common y standard plus1	2	246.182	246.148	0.034
beta common y standard plus1	3	375.224	375.046	0.178
beta xlink b standard plus3	3	640.336	640.458	-0.122
beta xlink b standard plus3	4	683.35	683.969	-0.619
beta xlink b standard plus4	3	480.504	480.609	-0.106
beta xlink b standard plus4	4	512.764	512.859	-0.094
beta xlink b standard plus4	5	537.531	537.666	-0.135
beta xlink y standard plus4	4	517.03	517.269	-0.239
beta xlink y standard plus4	5	545.301	545.448	-0.147
beta xlink y standard plus5	5	436.442	436.22	0.223

Figure S4.2. The MS/MS spectrum and the list of fragment ions of cross-linked peptide AKVQPYLDDFQKK-DLEEVK in human HDL



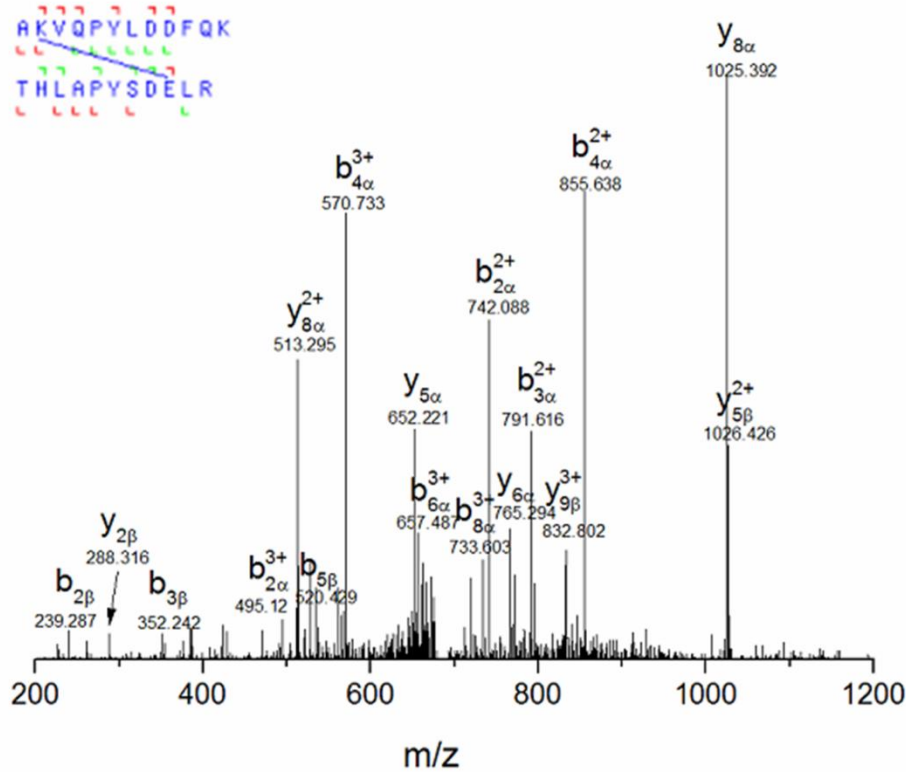
K96-E147, m/z: 616.82, Charge state: 4				
fragment type	position	ion th	peak	delta mz
alpha_common_y_standard_plus1	5	652.294	652.307	-0.013
alpha_common_y_standard_plus1	6	765.378	765.434	-0.056
alpha_common_y_standard_plus1	8	1025.494	1025.472	0.023
alpha_xlink_b_standard_plus2	2	606.824	607.084	-0.26
alpha_xlink_b_standard_plus2	3	656.359	656.495	-0.136
alpha_xlink_b_standard_plus2	4	720.388	720.537	-0.149
alpha_xlink_b_standard_plus2	6	850.446	850.579	-0.133
alpha_xlink_b_standard_plus3	11	773.388	773.668	-0.28
alpha_xlink_b_standard_plus3	4	480.595	480.535	0.06
alpha_xlink_b_standard_plus3	5	512.945	513.355	-0.409
alpha_xlink_b_standard_plus3	6	567.3	567.776	-0.476
alpha_xlink_b_standard_plus3	7	604.995	605.104	-0.11
alpha_xlink_b_standard_plus3	9	681.679	681.941	-0.262
alpha_xlink_y_standard_plus3	11	798.411	798.984	-0.573
alpha_xlink_y_standard_plus4	11	599.06	599.099	-0.039
beta_common_b_standard_plus1	2	201.124	201.013	0.111
beta_xlink_b_standard_plus3	7	720.373	720.537	-0.164
beta_xlink_b_standard_plus4	8	573.292	573.574	-0.283
beta_xlink_y_standard_plus3	4	666.332	666.287	0.044
beta_xlink_y_standard_plus3	7	755.385	755.59	-0.205
beta_xlink_y_standard_plus3	8	784.395	784.519	-0.123
beta_xlink_y_standard_plus4	5	514.256	514.503	-0.247
beta_xlink_y_standard_plus4	7	566.791	566.972	-0.182
beta_xlink_y_standard_plus4	8	588.549	588.894	-0.345

Figure S4.3. The MS/MS spectrum and the list of fragment ions of cross-linked peptide AKVQPYLDDFQK-LSPLGEEMR in human HDL



K96-D168, m/z: 447.92, Charge state: 6				
fragment type	Position	ion th	peak	delta mz
alpha_common_y_standard_plus2	4	275.672	275.666	0.006
alpha_common_y_standard_plus2	5	333.185	333.334	-0.149
alpha_common_y_standard_plus2	7	447.241	447.38	-0.14
alpha_common_y_standard_plus2	9	577.299	577.267	0.032
alpha_common_y_standard_plus3	6	260.802	260.724	0.077
alpha_common_y_standard_plus3	9	385.202	385.373	-0.172
alpha_xlink_b_standard_plus3	2	494.929	495.302	-0.374
alpha_xlink_b_standard_plus3	3	527.952	527.967	-0.016
alpha_xlink_b_standard_plus3	4	570.638	570.652	-0.014
alpha_xlink_b_standard_plus3	5	602.989	603.083	-0.094
alpha_xlink_b_standard_plus3	8	733.38	733.208	0.172
alpha_xlink_b_standard_plus4	13	711.873	711.795	0.078
alpha_xlink_b_standard_plus4	3	396.216	396.111	0.104
alpha_xlink_b_standard_plus4	4	428.23	428.266	-0.036
alpha_xlink_b_standard_plus4	6	493.259	493.421	-0.162
alpha_xlink_b_standard_plus4	7	521.53	521.273	0.257
alpha_xlink_b_standard_plus4	8	550.287	550.773	-0.486
alpha_xlink_b_standard_plus4	9	579.044	579.557	-0.513
beta_common_b_standard_plus1	2	239.114	239.221	-0.107
beta_common_b_standard_plus1	3	352.198	352.194	0.005
beta_common_b_standard_plus1	4	423.236	423.19	0.045
beta_common_b_standard_plus1	5	520.288	520.32	-0.032
beta_common_b_standard_plus2	6	342.18	342.177	0.003
beta_xlink_b_standard_plus4	10	672.848	673.339	-0.492
beta_xlink_b_standard_plus4	11	711.873	711.795	0.078
beta_xlink_b_standard_plus4	9	644.577	644.501	0.075
beta_xlink_y_standard_plus4	4	524.032	524.359	-0.327
beta_xlink_y_standard_plus4	5	545.79	545.989	-0.199
beta_xlink_y_standard_plus4	6	586.555	586.831	-0.275
beta_xlink_y_standard_plus4	7	610.819	611.026	-0.208
beta_xlink_y_standard_plus5	4	419.427	419.412	0.015
beta_xlink_y_standard_plus5	7	488.857	489.072	-0.215
beta_xlink_y_standard_plus5	9	525.681	525.543	0.137

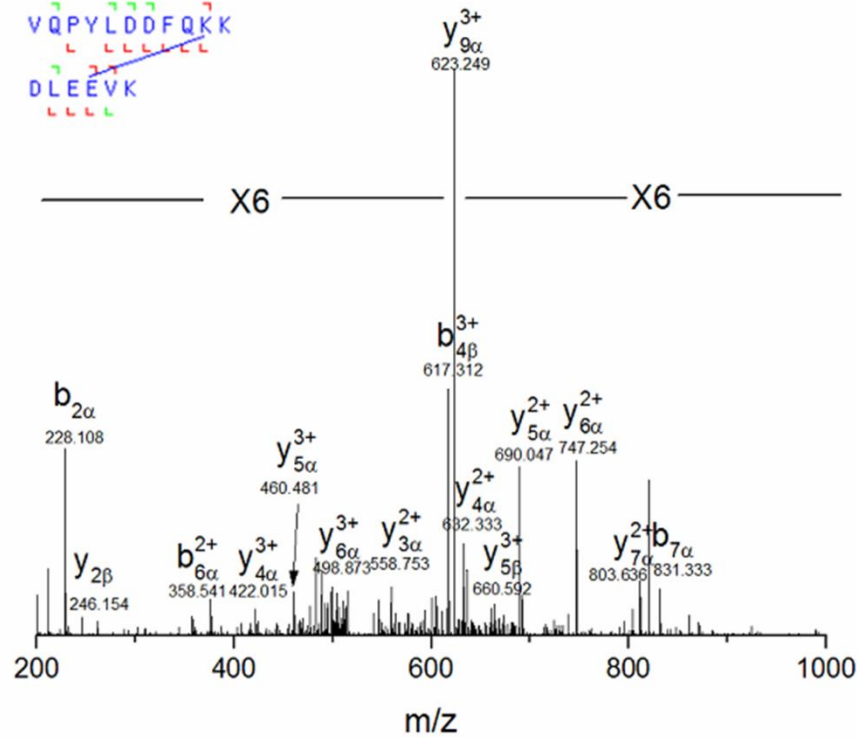
Figure S4.4. The MS/MS spectrum and the list of fragment ions of cross-linked peptide AKVQPYLDDFQK-THLAPYSDELR in human HDL



K96-E169, m/z: 684.351, Charge state: 4				
fragment type	position	ion th	peak	delta mz
alpha common y standard plus1	4	537.267	537.337	-0.07
alpha common y standard plus1	5	652.294	652.221	0.074
alpha common y standard plus1	6	765.378	765.294	0.084
alpha common y standard plus1	7	928.442	928.469	-0.028
alpha common y standard plus1	8	1025.494	1025.392	0.103
alpha common y standard plus2	8	513.251	513.295	-0.044
alpha common y standard plus2	9	577.28	577.4	-0.12
alpha xlink b standard plus2	2	741.889	742.088	-0.199
alpha xlink b standard plus2	3	791.423	791.616	-0.192
alpha xlink b standard plus2	4	855.453	855.638	-0.186
alpha xlink b standard plus3	2	494.929	495.12	-0.191
alpha xlink b standard plus3	3	527.952	528.102	-0.151
alpha xlink b standard plus3	4	570.638	570.733	-0.095
alpha xlink b standard plus3	6	657.343	657.487	-0.144
alpha xlink b standard plus3	8	733.38	733.603	-0.223
alpha xlink b standard plus3	9	771.722	771.621	0.101
alpha xlink y standard plus3	12	912.133	912.48	-0.347
alpha xlink y standard plus4	11	666.593	666.519	0.074
beta common b standard plus1	2	239.114	239.287	-0.172
beta common b standard plus1	3	352.198	352.242	-0.044
beta common b standard plus1	5	520.288	520.429	-0.14
beta common b standard plus1	7	770.384	770.225	0.159
beta common b standard plus1	8	885.411	885.333	0.078
beta common y standard plus1	2	288.204	288.316	-0.112
beta xlink b standard plus3	9	816.401	816.931	-0.53
beta xlink y standard plus2	5	1026.524	1026.426	0.098
beta xlink y standard plus3	11	912.133	912.48	-0.347
beta xlink y standard plus3	7	771.391	771.621	-0.231
beta xlink y standard plus3	8	795.07	795.332	-0.262
beta xlink y standard plus3	9	832.764	832.802	-0.038
beta xlink y standard plus4	5	513.766	513.985	-0.219
beta xlink y standard plus4	9	624.825	625.272	-0.447

Figure S4.5. The MS/MS spectrum and the list of fragment ions of cross-linked peptide AKVQPYLDDFQK-THLAPYSDEL R in human HDL

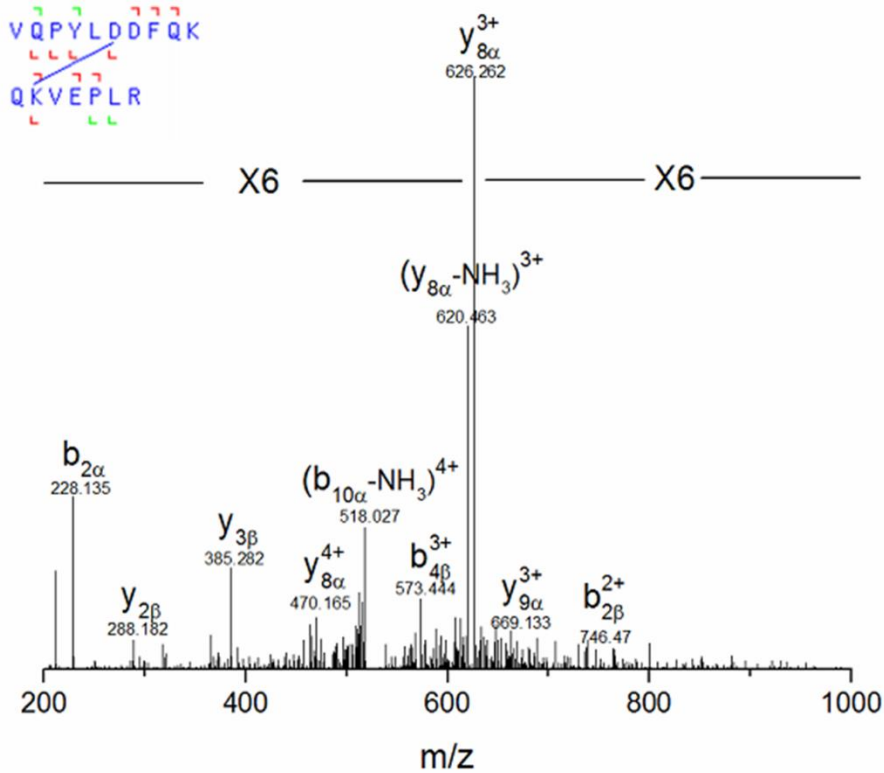
Cross-linking and MS/MS reveals multiple registries in APOA1



K106-E92, m/z: 524.276, Charge state: 4

fragment type	position	ion th	peak	delta mz
alpha_common_b_standard_plus1	2	228.135	228.108	0.027
alpha_common_b_standard_plus1	7	831.389	831.333	0.056
alpha_common_b_standard_plus2	6	358.685	358.541	0.144
alpha_common_b_standard_plus3	5	201.117	201.098	0.019
alpha_xlink_b_standard_plus4	10	487.748	487.784	-0.036
alpha_xlink_y_standard_plus2	2	494.788	494.744	0.044
alpha_xlink_y_standard_plus2	3	558.817	558.753,559.450	0.064,-0.633
alpha_xlink_y_standard_plus2	4	632.351	632.333,633.041	0.018,-0.689
alpha_xlink_y_standard_plus2	5	689.865	690.047	-0.183
alpha_xlink_y_standard_plus2	6	747.378	747.254,747.957	0.125,-0.579
alpha_xlink_y_standard_plus2	7	803.92	803.636,804.474	0.285,-0.554
alpha_xlink_y_standard_plus3	4	421.904	422.015	-0.111
alpha_xlink_y_standard_plus3	5	460.246	460.481	-0.235
alpha_xlink_y_standard_plus3	6	498.588	498.873	-0.285
alpha_xlink_y_standard_plus3	9	622.988	623.249	-0.261
beta_common_b_standard_plus1	2	229.119	229.119	0
beta_common_y_standard_plus1	2	246.182	246.154	0.027
beta_xlink_b_standard_plus3	4	616.973	617.312	-0.34
beta_xlink_b_standard_plus4	5	487.748	487.784	-0.036
beta_xlink_y_standard_plus3	3	579.646	579.715	-0.069
beta_xlink_y_standard_plus3	4	622.66	622.516,623.249	0.144,-0.589
beta_xlink_y_standard_plus3	5	660.355	660.592	-0.237
beta_xlink_y_standard_plus4	5	495.518	495.643	-0.125

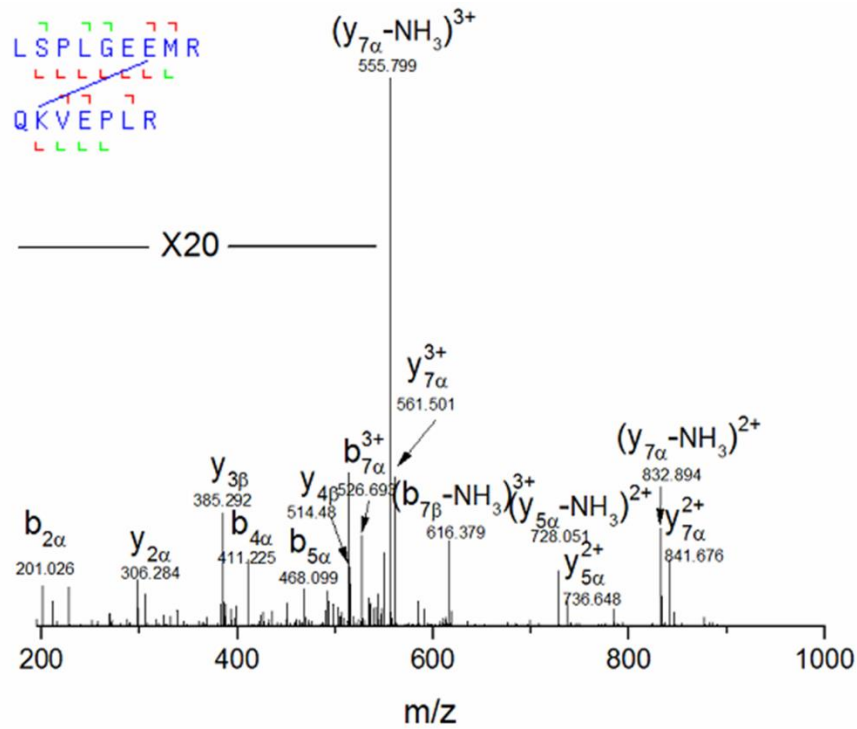
Figure S4.6. The MS/MS spectrum and the list of fragment ions of cross-linked peptide VQPYLDDFQKK-DLEEVK in human HDL



K118-D102, m/z: 526.538, Charge state: 4

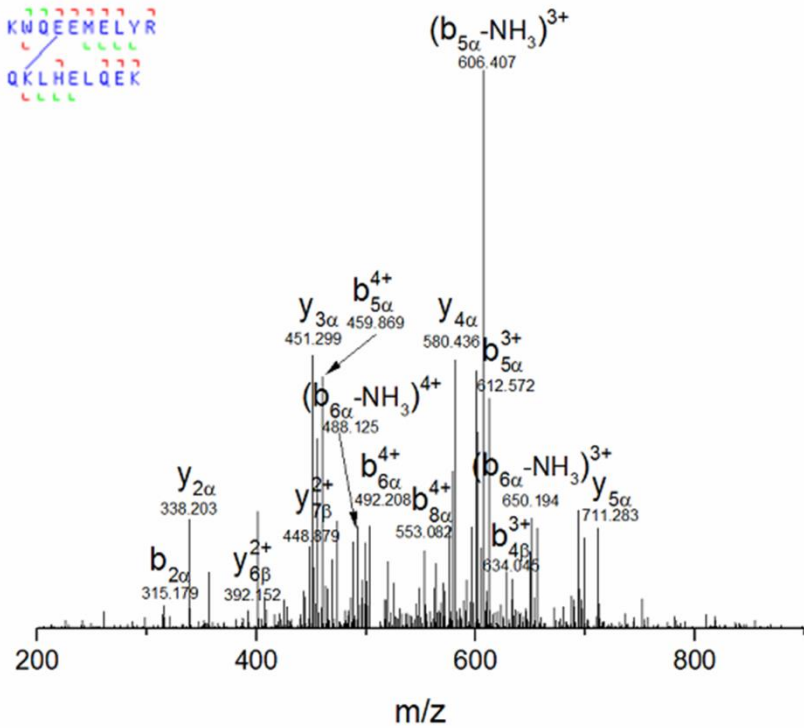
fragment type	position	ion th	peak	delta mz
alpha_common_b_standard_plus1	2	228.135	228.018	0.117
alpha_common_b_standard_plus1	4	488.251	488.347	-0.096
alpha_xlink_b_-NH3_plus4	10	517.778	518.027	-0.25
alpha_xlink_b_standard_plus3	7	561.302	561.827	-0.525
alpha_xlink_b_standard_plus4	8	457.996	457.814	0.182
alpha_xlink_b_standard_plus4	9	490.01	490.55	-0.54
alpha_xlink_y_-NH3_plus3	8	620.329	620.463	-0.134
alpha_xlink_y_standard_plus3	5	501.604	501.733	-0.129
alpha_xlink_y_standard_plus3	7	593.653	593.496	0.157
alpha_xlink_y_standard_plus3	8	626.004	626.262	-0.258
alpha_xlink_y_standard_plus3	9	668.69	669.133	-0.442
alpha_xlink_y_standard_plus4	8	469.755	470.165	-0.41
alpha_xlink_y_standard_plus4	9	501.77	501.733	0.037
beta_common_y_standard_plus1	2	288.204	288.182	0.022
beta_common_y_standard_plus1	3	385.256	385.282	-0.026
beta_xlink_b_standard_plus2	2	745.886	746.47	-0.584
beta_xlink_b_standard_plus3	4	573.63	573.444	0.186
beta_xlink_b_standard_plus3	5	605.981	606.399	-0.418
beta_xlink_y_standard_plus3	6	659.027	659.13	-0.103

Figure S4.7. The MS/MS spectrum and the list of fragment ions of cross-linked peptide VQPYLDDFQK-QKVEPLR in human HDL



K118-E147, m/z: 628.013 Charge state: 3				
fragment type	position	ion th	peak	delta mz
alpha_common_b_standard_plus1	2	201.124	201.026	0.098
alpha_common_b_standard_plus1	4	411.261	411.225	0.035
alpha_common_b_standard_plus1	5	468.282	468.099	0.184
alpha_common_y_standard_plus1	2	306.16	306.284	-0.124
alpha_xlink_b_standard_plus2	7	788.939	789.432	-0.493
alpha_xlink_b_standard_plus2	8	854.459	854.664	-0.205
alpha_xlink_b_standard_plus3	7	526.295	526.693	-0.398
alpha_xlink_y_-NH3_plus2	5	727.875	728.051	-0.176
alpha_xlink_y_-NH3_plus2	7	832.944	832.894,833.559	0.049,-0.615
alpha_xlink_y_-NH3_plus3	7	555.632	555.799	-0.167
alpha_xlink_y_standard_plus2	3	643.356	643.440,644.070	-0.084,-0.714
alpha_xlink_y_standard_plus2	4	707.878	707.867	0.01
alpha_xlink_y_standard_plus2	5	736.388	736.648	-0.26
alpha_xlink_y_standard_plus2	6	792.931	793.091	-0.16
alpha_xlink_y_standard_plus2	7	841.457	841.676	-0.219
alpha_xlink_y_standard_plus2	8	884.973	885.309	-0.336
alpha_xlink_y_standard_plus3	7	561.307	561.501	-0.193
alpha_xlink_y_standard_plus3	8	590.318	590.581	-0.263
beta_common_y_standard_plus1	3	385.256	385.292	-0.036
beta_common_y_standard_plus1	4	514.299	514.48	-0.181
beta_common_y_standard_plus1	5	613.367	613.431	-0.064
beta_xlink_b_-NH3_plus3	7	616.334	616.379	-0.045
beta_xlink_b_standard_plus2	3	684.869	685.26	-0.391
beta_xlink_b_standard_plus2	4	749.391	749.656	-0.265
beta_xlink_b_standard_plus2	6	854.459	854.664	-0.205
beta_xlink_y_standard_plus2	6	877.486	877.506	-0.021

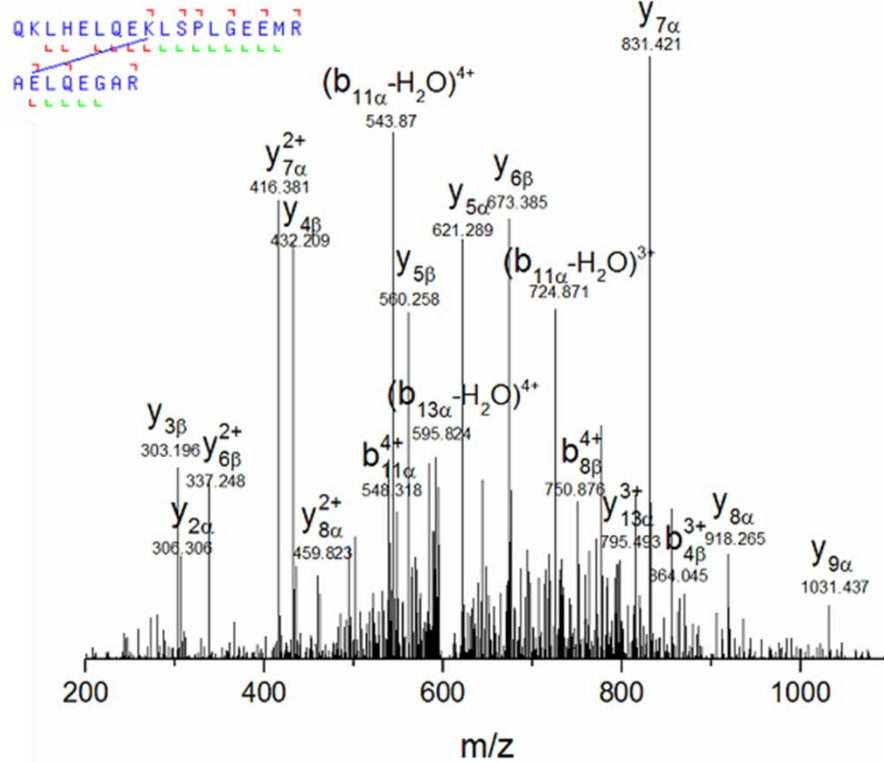
Figure S4.8. The MS/MS spectrum and the list of fragment ions of cross-linked peptide LSPLGEEMR-QKVEPLR in human HDL



K133-E110, m/z: 509.865, Charge state: 5

fragment type	position	ion th	peak	delta mz
alpha common b standard plus1	2	315.182	315.179	0.003
alpha common b standard plus1	3	443.241	443.182	0.059
alpha common y -NH3 plus1	5	694.323	694.36	-0.037
alpha common y standard plus1	2	338.183	338.203	-0.021
alpha common y standard plus1	3	451.267	451.299	-0.032
alpha common y standard plus1	4	580.309	580.436	-0.127
alpha common y standard plus1	5	711.35	711.283	0.067
alpha xlink b -NH3 plus3	5	606.645	606.407,607.029	0.238,-0.384
alpha xlink b -NH3 plus3	6	650.325	650.194,650.943	0.131,-0.618
alpha xlink b -NH3 plus4	6	487.996	488.125	-0.129
alpha xlink b standard plus3	4	569.306	569.786	-0.48
alpha xlink b standard plus3	5	612.32	612.572	-0.252
alpha xlink b standard plus3	6	656	656.364	-0.363
alpha xlink b standard plus3	7	699.015	699.343	-0.328
alpha xlink b standard plus4	10	632.575	632.645	-0.07
alpha xlink b standard plus4	4	427.232	427.523	-0.291
alpha xlink b standard plus4	5	459.492	459.869	-0.377
alpha xlink b standard plus4	6	492.252	492.208	0.045
alpha xlink b standard plus4	8	552.784	553.082	-0.298
alpha xlink y standard plus4	9	605.054	604.897,605.513	0.157,-0.459
alpha xlink y standard plus5	9	484.245	484.444	-0.199
beta common y -NH3 plus2	5	315.161	315.179	-0.018
beta common y standard plus1	5	646.341	646.372	-0.031
beta common y standard plus2	6	392.204	392.152	0.052
beta common y standard plus2	7	448.746	448.879	-0.133
beta xlink b standard plus3	4	633.99	634.045	-0.056
beta xlink b standard plus4	7	568.291	568.677	-0.386
beta xlink b standard plus4	8	600.551	600.811	-0.26
beta xlink b standard plus4	9	632.575	632.645	-0.07
beta xlink b standard plus5	8	480.643	481.049	-0.407
beta xlink y standard plus4	8	605.063	604.897,605.513	0.166,-0.450
beta xlink y standard plus5	8	484.252	484.444	-0.192

Figure S4.9. The MS/MS spectrum and the list of fragment ions of cross-linked peptide KWQEEMLYR-QKLHELQEK in human HDL



K140-E125, m/z:604.721, Charge state: 5

fragment type	position	ion th	peak	delta mz
alpha common y standard plus1	2	306.16	306.306	-0.146
alpha common y standard plus1	3	435.203	435.32	-0.117
alpha common y standard plus1	4	564.245	564.302	-0.057
alpha common y standard plus1	5	621.267	621.289	-0.022
alpha common y standard plus1	6	734.351	734.303	0.047
alpha common y standard plus1	7	831.403	831.421	-0.017
alpha common y standard plus1	8	918.435	918.265	0.17
alpha common y standard plus1	9	1031.52	1031.437	0.083
alpha common y standard plus2	7	416.206	416.381	-0.175
alpha common y standard plus2	8	459.722	459.823	-0.101
alpha xlink b -H2O plus3	11	724.391	724.871	-0.48
alpha xlink b -H2O plus4	11	543.545	543.87	-0.325
alpha xlink b -H2O plus4	13	596.079	595.824	0.255
alpha xlink b standard plus3	11	730.395	730.871	-0.476
alpha xlink b standard plus3	12	762.745	763.012	-0.267
alpha xlink b standard plus3	14	819.447	819.544	-0.097
alpha xlink b standard plus3	9	663.689	663.798	-0.109
alpha xlink b standard plus4	11	548.048	548.318	-0.271
alpha xlink b standard plus4	18	751.144	750.876,751.690	0.268,-0.545
alpha xlink b standard plus5	16	543.689	543.87	-0.182
alpha xlink y standard plus3	10	672.018	672.504	-0.485
alpha xlink y standard plus3	11	715.032	715.429	-0.397
alpha xlink y standard plus3	13	795.413	795.493	-0.08
alpha xlink y standard plus4	12	568.541	568.397	0.144
alpha xlink y standard plus4	15	663.337	663.798	-0.461
alpha xlink y standard plus4	16	691.608	692.11	-0.502
beta common y standard plus1	3	303.178	303.196	-0.018
beta common y standard plus1	4	432.221	432.209	0.012
beta common y standard plus1	5	560.279	560.258	0.021
beta common y standard plus1	6	673.363	673.385	-0.022
beta common y standard plus2	6	337.186	337.248	-0.062
beta xlink b standard plus3	2	783.075	783.151	-0.077
beta xlink b standard plus3	4	863.455	864.045	-0.589
beta xlink b standard plus4	2	587.558	587.824	-0.266
beta xlink b standard plus4	4	647.844	647.833	0.01
beta xlink b standard plus4	8	751.144	750.876,751.690	0.268,-0.545
beta xlink y standard plus5	7	590.512	590.921	-0.41

Figure S4.10. The MS/MS spectrum and the list of fragment ions of cross-linked peptide QKLHELQEKLSPLGEEMR-AELQEGAR in human HDL