SUPPLEMENTARY INFORMATION

Table S1

The HX time-courses (pD 7.3, 5°C) of 51 lipid-free apoA-I_{WT} and apoA-I_{Iowa} peptide fragments were fitted with one or two exponentials and the estimated protection factors (Pf) are tabulated. Because the different hydrogens in a given segment have a range of unprotected HX rates, the curves are drawn to fit a stretched exponential (stretching factor ~0.8). If the best-fit is a mono-exponential equation there is one protection factor and if the best-fit is a bi-exponential equation there are two protection factors, one for the fast initial phase (Phase I) and one for the second slower phase (Phase II). The overall Pf for such fragments is calculated as an average of the two values weighted for the number of residues in each phase. Certain apoA-I_{Iowa} peptides (residues 17-46, 114-126 and 127-158) give rise to bimodal mass spectra (Fig. S1). The two populations exhibiting fast and slow HX kinetics are analyzed separately and designated as "fast" and "slow" in the table. The Pf values for these peptides are derived from time-courses of deuterium incorporation like those shown in Fig. 2b. The Pf can be underestimated in cases where the EX1 contribution to HX is calculated as EX2 behavior.

Table S1

Residues	Total amides	Fast residues	Slow residues	Intrinsic Rate	Stretch-factor	pf(I)	pf(II)
WT:3-16	11	6	5	22.0	0.83	13	3826
Iowa:3-16	11	--	--	22.0	0.83	15	--
WT:3-17	12	6	6	21.0	0.83	12	4622
Iowa:3-17	12	11	1	21.0	0.83	15	--
WT:17-32	14	3	11	22.5	0.71	15	1524
Iowa:17-32	14	--	--	22.5	0.71	16	--
WT:17-46	28	14	14	27.1	0.74	35	1556
Iowa:17-46 (slow)	28	14	14	27.1	0.74	34	--
Iowa:17-46 (fast)	28	14	14	27.1	0.74	10	--
WT:34-44	9	5	4	40.1	0.77	40	678
Iowa:34-44	9	--	--	40.1	0.77	21	--
WT:34-46	11	6	5	33.8	0.77	24	509
Iowa:34-46	11	--	--	33.8	0.77	25	--
WT:45-56	10	--	--	28.0	0.73	7	--
Iowa:45-56	10	--	--	27.9	0.73	5	--
WT:51-60	8	6	2	42.4	0.76	12	5311
Iowa:51-60	8	--	--	42.4	0.76	4	--
WT:51-71	18	10	8	29.0	0.79	15	3023
Iowa:51-71	18	8	10	29.0	0.79	4	87
WT:61-71	8	4	4	21.7	0.83	21	3319
Iowa:61-71	8	3	5	21.7	0.83	4	70
WT:72-89	16	6	10	29.6	0.82	62	9856
Iowa:72-89	16	10	6	29.6	0.82	31	393
WT:72-91	18	6	12	24.7	0.79	31	9037
Iowa:72-91	18	11	7	24.7	0.79	22	344
WT:72-92	19	6	13	23.2	0.79	43	9226
Iowa:72-92	19	12	7	23.2	0.79	16	332
WT:72-103	29	8	21	20.7	0.81	46	9327
Iowa:72-103	29	15	14	20.7	0.81	60	839
WT:76-89	12	4	8	32.5	0.84	34	12917
Iowa:76-89	12	7	5	32.5	0.84	30	393
WT:76-91	14	4	10	25.2	0.80	34	13905
Iowa:76-91	14	8	6	25.2	0.80	23	429
WT:76-92	15	5	10	23.3	0.79	16	14026
Iowa:76-92	15	9	6	23.3	0.79	19	361
WT:76-103	25	6	19	20.4	0.81	18	11768
Iowa:76-103	25	11	14	20.4	0.81	36	756
WT:90-103	11	4	7	15.9	0.87	121	4190
Iowa:90-103	11	4	7	15.9	0.87	90	871

Residues	Total amides	Fast residues	Slow residues	Intrinsic Rate	Stretch-factor	pf(I)	pf(II)
WT:92-103	9	2	7	19.2	0.89	226	11237
Iowa:92-103	9	--	--	19.2	0.89	547	--
WT:92-104	10	1	9	18.9	0.89	16	7663
Iowa:92-104	10	3	7	18.9	0.89	81	875
WT:93-103	8	1	7	18.4	0.88	13	6240
Iowa:93-103	8	4	4	18.4	0.88	144	1237
WT:93-104	9	1	8	18.1	0.89	7	6423
Iowa:93-104	9	2	7	18.1	0.89	18	764
WT:96-103	5	1	4	15.5	0.95	0	6295
Iowa:96-103	5	--	--	15.5	0.95	276	--
WT:104-113	8	1	7	24.6	0.88	8	6958
Iowa:104-113	8	--	--	24.6	0.88	2001	--
WT:104-114	9	1	8	21.3	0.86	0	3568
Iowa:104-114	9	1	8	21.3	0.86	0	1577
WT:114-124	8	--	--	23.4	0.73	15	--
Iowa:114-124 (slow)	8	--	--	23.4	0.73	468	--
Iowa:114-124 (fast)	8	--	--	23.4	0.73	15	--
WT:114-126	10	--	--	19.2	0.74	10	--
Iowa:114-126 (slow)	10	--	--	19.2	0.74	240	--
Iowa:114-126 (fast)	10	--	--	19.2	0.74	8	--
WT:125-158	31	24	7	30.7	0.80	8	6384
Iowa:125-158 (slow)	31	23	8	30.7	0.80	6	613
Iowa:125-158 (fast)	31	--	--	30.7	0.80	6	--
WT:127-158	29	22	7	31.1	0.79	7	5387
Iowa:127-158 (slow)	29	--	--	31.1	0.79	623	--
Iowa:127-158 (fast)	29	21	8	31.1	0.79	6	623
WT:155-169	12	4	8	28.2	0.75	22	12157
Iowa:155-169	12	8	4	28.2	0.75	29	1030
WT:159-169	8	2	6	35.8	0.70	30	7295
Iowa:159-169	8	5	3	35.8	0.70	27	645
WT:159-170	9	2	7	28.8	0.68	15	8652
Iowa:159-170	9	4	5	28.8	0.68	16	308
WT:159-174	13	2	11	31.8	0.72	224	15603
Iowa:159-174	13	5	8	31.8	0.72	31	851
WT:159-176	15	3	12	31.8	0.74	9	7312
Iowa:159-176	15	5	10	31.8	0.74	21	792
WT:159-180	19	2	17	28.6	0.76	19	12024
Iowa:159-180	19	8	11	28.6	0.76	82	1064
WT:160-169	7	1	6	33.7	0.69	6	4946
Iowa:160-169	7	4	3	33.7	0.69	18	784

Residues	Total amides	Fast residues	Slow residues	Intrinsic Rate	Stretch-factor	pf(I)	pf(II)
WT:179-189	9	9	--	37.2	0.74	7	--
Iowa:179-189	9	9	--	37.2	0.74	6	--
WT:190-213	21	--	--	33.29	0.77	1	--
Iowa:190-213	21	--	--	33.2	0.77	1	--
WT:212-219	6	--	--	20.4	0.68	9	--
Iowa:212-219	6	--	--	20.4	0.68	6	--
WT:212-222	8	--	--	14.1	0.68	7	--
Iowa:212-222	8	--	--	14.1	0.68	5	--
WT:212-225	11	--	--	16.4	0.69	3	--
Iowa:212-225	11	--	--	16.4	0.69	4	--
WT:213-222	7	--	--	16.0	0.67	8	--
Iowa:213-222	7	--	--	16.0	0.67	6	--
WT:213-225	10	--	--	18.2	0.68	5	--
Iowa:213-225	10	--	--	18.2	0.68	5	--
WT:214-222	6	--	--	14.2	0.64	8	--
Iowa:214-222	6	--	--	14.2	0.64	6	--
WT:214-225	9	--	--	17.1	0.66	6	--
Iowa:214-225	9	--	--	17.1	0.66	7	--
WT:215-225	8	--	--	14.8	0.68	4	--
Iowa:215-225	8	--	--	14.8	0.68	4	--
WT:226-232	5	--	--	42.1	0.80	23	--
Iowa:226-232	5	--	--	42.1	0.80	14	--
WT:233-243	9	--	--	26.9	0.78	10	--
Iowa:233-243	9	--	--	26.9	0.78	9	--
WT:234-243	8	--	--	31.8	0.81	12	--
Iowa:234-243	8	--	--	31.8	0.81	11	--
WT:236-243	6	--	--	35.3	0.79	12	--
Iowa:236-243	6	--	--	35.3	0.79	11	--

Table S2

The HX time-courses (pD 7.3, 5°C) of 41 lipid-free apoA-I_{WT} and apoA-I_{Mil} peptide fragments were analyzed as described in Table S1.

Table S2

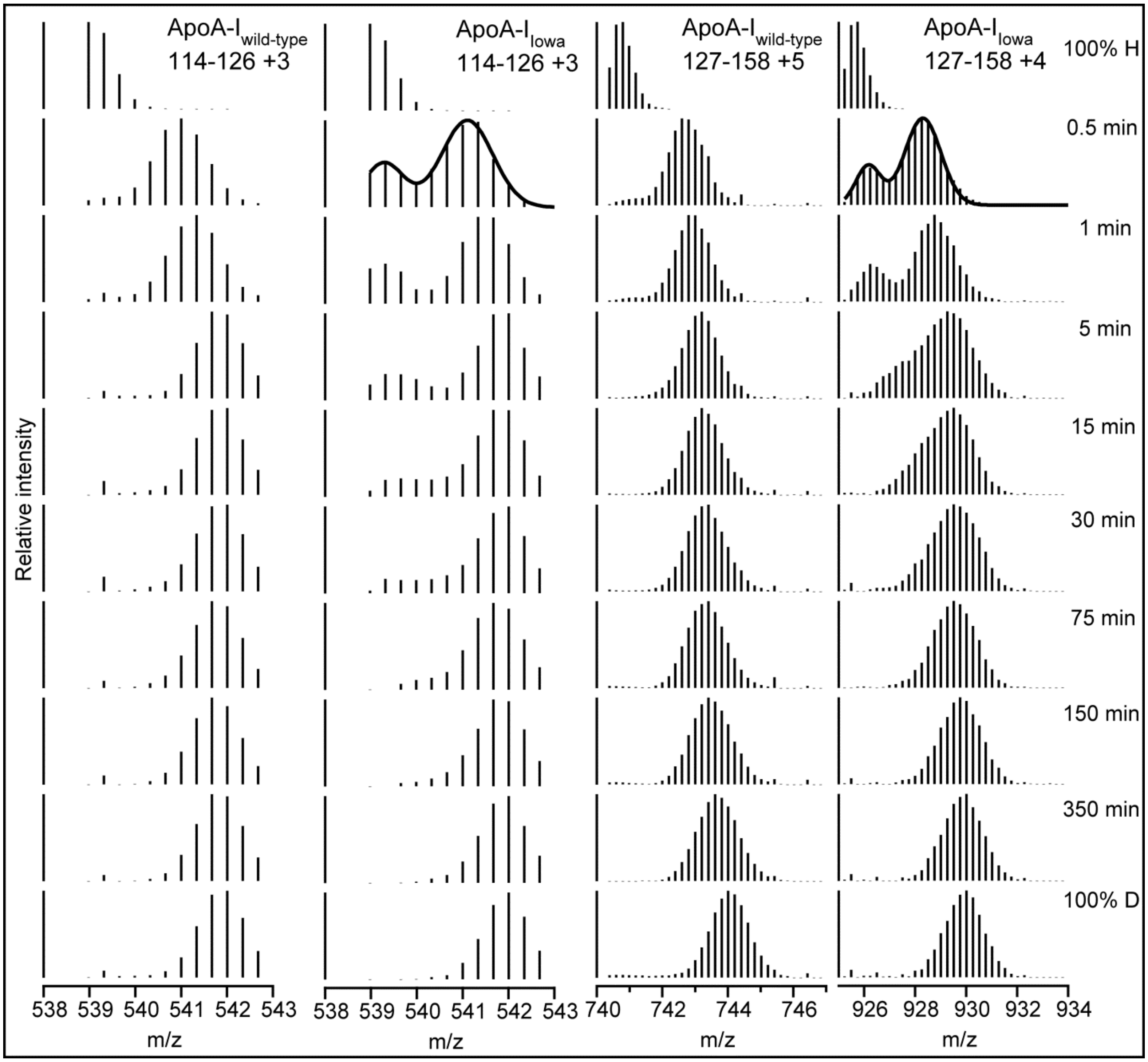
Residues	Total amides	Fast residues	Slow residues	Intrinsic Rate	Stretch-factor	pf(I)	pf(II)
Milano: -2-16	11	7	5	19.8	0.80	5	980
WT:17-46	28	14	14	27.1	0.74	35	1556
Milano:17-46(slow)	28	18	10	27.1	0.74	24	1946
Milano:17-46(Fast)	28	20	8	27.1	0.74	1	22
WT:19-46	26	14	12	29.3	0.74	34	1757
Milano:19-46(slow)	26	15	11	29.3	0.74	31	2429
Milano:19-46(Fast)	26	26		29.3	0.74	6	--
WT:29-46	16	8	8	36.3	0.78	28	728
Milano:29-46(slow)	16	9	7	36.3	0.78	24	1639
Milano:29-46(Fast)	16	15	1	36.3	0.78	4	94
WT:47-56	8	8		40.4	0.79	6	--
Milano:47-56	8	8		40.4	0.79	5	--
WT:51-71	18	10	8	29.0	0.79	15	3023
Milano:51-71 (Slow)	18	8	10	29.0	0.79	16	4911
Milano:51-71 (Fast)	18	12	6	29.0	0.79	1	60
Milano:57-70(slow)	11	6	5	24.1	0.83	198	5438
Milano:57-70(Fast)	11	11		24.1	0.83	12	--
WT:61-71	8	4	4	21.7	0.83	21	3319
Milano:61-71(slow)	8	5	3	21.7	0.83	20	4143
Milano:61-71(Fast)	8	6	2	21.7	0.83	1	321
WT:72-103	29	8	21	20.7	0.81	46	9327
Milano:72-103(slow)	29	23	6	20.7	0.81	132	13547
Milano:72-103(Fast)	29	19	10	20.7	0.81	1	241
WT:104-113	8	1	7	24.6	0.88	8	6958
Milano:104-113	8	5	3	24.6	0.88	868	8373
WT:114-126	10	10	--	19.2	0.74	10	--
Milano:114-126 (slow)	10	8	2	19.2	0.74	89	769
Milano:114-126 (Fast)	10	8	2	19.2	0.74	5	155
WT:125-158	31	24	7	30.7	0.80	8	6384
Milano:125-158 (slow)	31	3	28	30.7	0.80	1	1813
Milano:125-158 (Fast)	31	22	9	30.7	0.80	6	6091
WT:159-169	8	2	6	35.8	0.70	30	7295
Milano:159-169 (slow)	8	8	--	35.8	0.70	13754	--
Milano:159-169 (Fast)	8	6	2	35.8	0.70	4	3584
Milano:170-174	3	3	--	44.9	0.80	24734	--
Milano:175-189	13	6	7	30.0	0.75	4	24997
WT:179-202	22	22	--	41.0	0.76	9	--
Milano:179-202	22	22	--	41.0	0.76	5	--
WT:181-189	7	7	--	53.0	0.79	7	--

Residues	Total amides	Fast residues	Slow residues	Intrinsic Rate	Stretch-factor	pf(I)	pf(II)
Milano:181-189	7	7	--	53.0	0.79	6	--
WT:203-213	8	8	--	20.3	0.88	7	--
Milano:203-213	8	--	--	20.3	0.88	8	--
WT:214-225	9	9	--	17.1	0.66	6	--
Milano:214-225	9	--	--	17.1	0.66	6	--
Milano:226-233	6	--	--	31.5	0.75	5	--
WT:236-243	6	--	--	35.3	0.79	12	--
Milano:233-243	9	--	--	26.9	0.78	9	--

Figure S1

Comparison of the mass spectra for apoA-I_{WT} and apoA-I_{Iowa} peptide fragments 114-126 (charge state +3) and 127-158 (charge state +4 or +5). Isotopic envelopes at different times of deuterium (D) incorporation together with the spectrum of the fully deuterated peptide are shown. The apoA-I_{WT} spectra are unimodal but the apoA-I_{Iowa} spectra are bimodal. In the latter case where mixed EX1/EX2 HX kinetics occur, the peptide contains two populations of amide hydrogens with fast and slow HX rates and different degrees of incorporation of D. To estimate the fraction of the population in the HX time point samples, the mass spectra were fitted by non-linear regression to a double Gaussian equation (solid line in 0.5 min spectrum) and integrated to obtain peak intensities.

Figure S1



ApoA-I wild-type 114-126 +3
ApoA-I Iowa 114-126 +3
ApoA-I wild-type 127-158 +5
ApoA-I Iowa 127-158 +4
100% H
0.5 min
1 min
5 min
15 min
30 min
75 min
150 min
350 min
100% D
Relative intensity
538 539 540 541 542 543
m/z
538 539 540 541 542 543
m/z
740 742 744 746
m/z
926 928 930 932 934
m/z