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Simulated quantitative and qualitative isotachophoretic indices of 73 amino acids and peptides in the pH range 6.4–10

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ABSTRACT

Qualitative and quantitative isotachophoretic indices of 73 amino acids, dipeptides and tripeptides were simulated under 24 leading electrolyte conditions covering the pH range 6.4–10. The R_E values and time-based zone lengths are tabulated together with the absolute mobility (m_0) and pK_a values used. The leading electrolyte used was 10 m*M* HCl and the pH buffers were imidazole, tris(hydroxymethylamino)methane, 2-amino-2-methyl-1,3-propanediol and ethanolamine. The simulated indices will be useful in the assessment of the separability and determination of the listed and related compounds.

INTRODUCTION

In 1983 we published qualitative and quantitative isotachophoretic (ITP) indices for 287 ions in the pH range 3–10 in a tabular form [1]. The validity of the simulation has been confirmed for many samples. For example, Oefner *et al.* [2] measured qualitative and quantitative indices of 52 anions and compared them with the simulated values and correlation factors of 0.993 and 0.92 were obtained for qualitative and quantitative indices, respectively. In addition to this extensive comparative work, many researchers have utilized the table for separability assessment.

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In this work, the qualitative and quantitative ITP indices of 73 amino acids and peptides as anions were simulated on the basis of the absolute mobilities and thermodynamic dissociation constants. Most of them have been evaluated by the ITP technique [3–5] and several of them were refined using new R_E data. The methods used for the evaluation of physico-chemical constants have been reviewed by Pospichal *et al.* [6].

SIMULATION

Method

The simulation techniques were the same as in the previous work [1]; iterative calculation using the RFQ method [7] was carried out to fulfil ITP conditions. The effect of ionic strength on the mobilities and dissociation constants was considered.

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TABLE I

ELECTROLYTE SYSTEMS USED IN SIMULATION FOR AN ANIONIC ANALYSIS

Leading ion = 10 m*M* Cl^-. Gly-Gly = glycylglycine; β-Ala = β-alanine; ε-AMC = ε-aminocaproic acid; CR = creatinine; HIS = histidine; IM = imidazole; TRIS = tris(hydroxymethylamino)methane (Tris); AMEDIOL = 2-amino-2-methyl-1,3-propanediol; EA anolamine.

Buffers	Number and the pH of leading solutions						
Gly-Gly	(1)2.6	(2)2.8	(3)3.0	(4)3.2	(5)3.4	(6)3.6	
β-Ala	(7)3.0	(8)3.2	(9)3.4	(10)3.6	(11)3.8	(12)4.0	
ε-AMC	(13)3.8	(14)4.0	(15)4.2	(16)4.4	(17)4.6	(18)4.8	
CR	(19)4.2	(20)4.4	(21)4.6	(22)4.8	(23)5.0	(24)5.2	(25)5.4
HIS	(26)5.4	(27)5.6	(28)5.8	(29)6.0	(30)6.2	(31)6.4	
IM	(32)6.4	(33)6.6	(34)6.8	(35)7.0	(36)7.2	(37)7.4	
TRIS	(38)7.4	(39)7.6	(40)7.8	(41)8.0	(42)8.2	(43)8.4	
AMEDIOL	(44)8.2	(45)8.4	(46)8.6	(47)8.8	(48)9.0	(49)9.2	
EA	(50)9.0	(51)9.2	(52)9.4	(53)9.6	(54)9.8	(55)10.	

Electrolyte system

The leading electrolyte was 10 m*M* HCl containing an appropriate pH buffer. The pH range of the leading electrolyte (pH_L) was varied in the range of 6.4–10 (0.2 pH steps, electrolytes 32–55) using four different pH buffers as shown in Table I. For a few acidic amino acids, the pH range was 3–10 and eight kinds of buffers were used (electrolytes 1–55).

TABLE II

SIMULATED EFFECTIVE MOBILITIES AND CONCENTRATIONS OF LEADING ZONE CONSTITUENTS

Leading ion = 10 m*M* Cl^-. pH_L = pH of leading electrolyte; m_L = effective mobility of leading ion (10^{-5} cm^2 V^{-1} s^{-1}); $C^t_{B,L}$ = total concentration (m*M*) of buffer ion; $m_{B,L}$ = effective mobility of buffer ion (10^{-5} cm^2 V^{-1} s^{-1}); R_L = specific resistance of leading electrolyte (Ω m); E_L = potential gradient of leading zone (V cm^{-1}); v = isotachophoretic velocity (10^{-3} cm s^{-1}). Capillary I.D. = 0.5 mm.

Buffer	pH_L	m_L	$C^t_{B,L}$	$m_{B,L}$	R_L	E_L	v
IM	(32) 6.4	−74.70	11.60	41.51	8.435	42.96	32.09
	(33) 6.6	−74.70	12.54	38.41	8.435	42.96	32.09
	(34) 6.8	−74.70	14.03	34.34	8.435	42.96	32.09
	(35) 7.0	−74.70	16.38	29.40	8.435	42.96	32.09
	(36) 7.2	−74.70	20.12	23.94	8.435	42.96	32.09
	(37) 7.4	−74.70	26.03	18.50	8.435	42.96	32.09
TRIS	(38) 7.4	−74.70	11.90	21.95	10.28	52.35	39.11
	(39) 7.6	−74.70	13.01	20.07	10.28	52.35	39.10
	(40) 7.8	−74.70	14.78	17.68	10.28	52.35	39.10
	(41) 8.0	−74.70	17.57	14.87	10.28	52.34	39.10
	(42) 8.2	−74.70	22.00	11.88	10.28	52.33	39.09
	(43) 8.4	−74.70	29.02	9.00	10.27	52.33	39.09
AMEDIOL	(44) 8.2	−74.70	12.37	23.10	10.03	51.10	38.17
	(45) 8.4	−74.70	13.76	20.77	10.03	51.09	38.16
	(46) 8.6	−74.70	15.96	17.91	10.03	51.07	38.15
	(47) 8.8	−74.70	19.45	14.70	10.02	51.04	38.13
	(48) 9.0	−74.70	24.99	11.45	10.01	51.00	38.10
	(49) 9.2	−74.70	33.77	8.47	10.00	50.94	38.05
EA	(50) 9.0	−74.69	12.88	31.58	8.969	45.68	34.12
	(51) 9.2	−74.69	14.56	27.94	8.959	45.63	34.08
	(52) 9.4	−74.69	17.24	23.62	8.942	45.54	34.01
	(53) 9.6	−74.69	21.49	18.98	8.915	45.41	33.91
	(54) 9.8	−74.68	28.24	14.47	8.874	45.19	33.75
	(55) 10.0	−74.69	39.01	10.51	8.808	44.86	33.50

TABLE III

PHYSICO-CHEMICAL CONSTANTS OF BUFFERS USED IN SIMULATIONS (25°C)

m_0 = Absolute mobility ($cm^2\ V^{-1}\ s^{-1}$); pK_a = thermodynamic dissociation constant.

Buffer	m_0	pK_a
Gly-Gly	31.5	3.140
β-ala	36.7	3.552
ε-AMC	28.8	4.373
CR	37.2	4.828
HIS	29.6	6.040
IM	52.0	7.150
TRIS	29.5	8.076
AMEDIOL	29.5	8.780
EA	44.3	9.498
Cl^-	79.1	–

Table II summarizes the simulated effective mobilities and concentrations of the leading zone constituents. Table III gives the absolute mobilities and thermodynamic dissociation constants of the buffers used. Most of them were obtained by ITP but some were taken from the literature [8–11]. The names and abbreviations of substances treated are given in Table IV.

Migration conditions

The inner diameter of the separation tube was 0.5 mm, the migration current was 100 μA and the temperature of the separation tube was 25°C.

CONTENTS OF SIMULATED DATA

The contents of the simulated data given in Table V, pH_L, pH_S, m, R_E, t, R_S and IS, are explained briefly below.

pH_L

This is the pH of the leading electrolyte used in the simulation. The leading electrolytes used are summarized in Table I. Eight different buffers were used to adjust the pH of 10 m*M* HCl. To maintain a good buffering capacity of the leading electrolyte, the pH_L should satisfy the relationship $pK_Q - 0.5 < pH_L < pK_Q + 0.5$, where pK_Q is the pK_a of the buffers used. The maximum buffering capacity is obtained at $pH_L = pK_Q$.

pH_S

This is the pH of the sample zone at the steady state evaluated by simulation. When pH_S differs significantly from pH_L (approximately over 1–1.5), the

TABLE IV

NAMES OF SAMPLES AND ABBREVIATIONS USED

No.[a]	Name	Abbreviation
400	Alanylalanine	Ala-Ala
401	L-Alanyl-L-alanyl-L-alanine	Ala-Ala-Ala
402	Alanyl-α-amino-*n*-butyric acid	Ala-Amin
403	Alanylasparagine	Ala-Asn
404	Alanylglycine	Ala-Gly
405	DL-Alanylglycylglycine	Ala-Gly-Gly
406	β-Alanylhistidine	β-Ala-His
407	Alanylleucine	Ala-Leu
408	DL-Alanyl-DL-leucylglycine	Ala-Leu-Gly
409	Alanylmethionine	Ala-Met
410	β-Alanine	β-Ala
411	Alanine	Ala
412	Alanylphenylalanine	Ala-Phe
413	Alanylserine	Ala-Ser
414	Alanylvaline	Ala-Val
415	α-Amino-*n*-nutyric acid	Amin
417	Asparagine	Asn
418	Aspartic acid	Asp
419	Cysteine	Cys
420	Cystine	CysH

(Continued on p. 286)

TABLE IV *(continued)*

No.[a]	Name	Abbreviation
421	Glutamic acid	Glu
422	Glutamine	Gln
423	Glycylalanine	Gly-Ala
424	Glycyl-α-amino-*n*-butyric acid	Gly-Amin
425	Glycylasparagine	Gly-Asn
426	Glycine	Gly
427	Diglycine	Gly-Gly
428	Triglycine	Gly-Gly-Gly
429	Tetraglycine	Gly-Gly-Gly-Gly
430	Pentaglycine	Gly-Gly-Gly-Gly-Gly
431	Hexaglycine	Gly-Gly-Gly-Gly-Gly-Gly
432	Glycylglycyl-L-isoleucine	Gly-Gly-Ile
433	Glycylglycyl-D-leucine	Gly-Gly-Leu
434	Glycylglycyl-L-phenylalanine	Gly-Gly-Phe
435	Glycylglycyl-L-valine	Gly-Gly-Val
436	Glycyl-L-histidylglycine	Gly-His-Gly
437	Glycylisoleucine	Gly-Ile
438	Glycyl-L-leucine	Gly-Leu
439	Glycyl-DL-leucyl-DL-alanine	Gly-Leu-Ala
440	Glycyl-L-leucyl-L-tyrosine	Gly-Leu-Tyr
441	Glycylphenylalanine	Gly-Phe
442	Glycyl-L-phenylalanyl-L-phenylalanine	Gly-Phe-Phe
443	Glycyl-L-proline	Gly-Pro
444	Glycyl-L-prolyl-L-alanine	Gly-Pro-Ala
445	Glycylserine	Gly-Ser
446	Glycyl-D-threonine	Gly-Thr
447	Glycyltryptophane	Gly-Trp
448	Glycyltyrosine	Gly-Tyr
449	Glycylvaline	Gly-Val
450	Histidine	His
451	Hydroxyproline	Hyp
452	Isoleucine	Ile
453	Leucine	Leu
454	Leucylglycine	Leu-Gly
455	L-Leucylglycylglycine	Leu-Gly-Gly
456	DL-Leucylglycyl-DL-phenylalananine	Leu-Gly-Phe
457	Leucylleucine	Leu-Leu
458	L-Leucyl-L-leucyl-L-leucine	Leu-Leu-Leu
459	Leucylphenylalanine	Leu-Phe
460	L-Leucyl-L-tyrosine	Leu-Tyr
461	Leucylvaline	Leu-Val
463	Methionine	Methionine
464	Ornithine	Ornithine
465	Phenylalanine	Phenylalanine
466	Proline	Proline
467	Serine	Serine
468	L-Seryl-L-seryl-L-serine	Ser-Ser-Ser
469	Taurine	Taurine
470	Threonine	Threonine
471	Tryptophan	Tryptophan
472	Tyrosine	Tyrosine
473	Valine	Valine
474	3,5-Diiodotyrosine	I2-Tyr

[a] In our database, 416 and 462 correspond to arginine and lysine, respectively. As they are cations in the pH range 6.4–10, they are not included here.

buffering ability of the counter ion might not be so good and also the experimental reproducibility of R_E and R_s may not be good.

m_S

This is the effective mobility of the sample at the steady state 10^{-5} cm^2 V^{-1} s^{-1}. When the effective mobility of the sample is very small, the pH shift is very large and therefore the isotachophoretic migration may be unstable.

R_E

The ratios of potential gradients can be qualitative indices of the separated zones. R_E is one of the qualitative indices, defined as

$$R_E = E_S/E_L = m_L/m_S = R_S/R_L \ (= h_S/h_L)$$

where E, m, R and h denote the potential gradient, the effective mobility, the specific resistance and the step height in the recorder trace, respectively, and the subscripts L and S denote the leading and sample zones, respectively. In order to convert the step heights into R_E values, the step heights of the leading zones, h_L, should be estimated by the equation

$$h_L = h_{std}/(R_{E,std} - 1)$$

where h_{std} is the observed step height of a standard sample for the conversion and $R_{E,std}$ is the R_E value of the standard. It should be noted that a linear relationship is assumed between step heights and potential gradients. The identification power of isotachophoresis using qualitative R_E indices has been confirmed theoretically by Kenndler [12].

t

This is the time-based zone length of a 10-nmol sample in seconds. As the migration current was 100 μA, it corresponds to the electric charge in 10^{-4}C; for t = 28.65 s, it means that the zone length of a 10-nmol sample will be 28.65 s when a migration current of 100 μA is applied and the electric charge will be 2.865 mC. This might be useful for estimating the time-based zone length when the migration current is different from 100 μA.

R_S

This is the ionic specific resistance of the separated zones in Ω m. This parameter is newly added based on the wide use of conductivity detectors.

IS

This is the strength of the separated zones in mM. When the migration order of the zones is simulated, the effective mobility of the ith ion in the jth zone ($m_{i,j}$) and that of the jth ion in the ith zone ($m_{j,i}$) should be evaluated and compared [13,14]. The ionic strength is necessary in the correction of absolute mobility.

TABLE V

ISOTACHOPHORETIC INDICES OF 73 AMINO ACIDS AND PEPTIDES

The first line for each sample shows the following information:

No.	Chemical formula	Abbreviation	m_0	pK_a	Relative molecular mass
400	$C_6H_{12}N_2O_3$	Ala-Ala	−27.0	8.490	160.2

pH_L = pH of the leading electrolyte used in simulation; pH_S = pH of the sample zone at the steady state; m_S = effective mobility of the sample at the steady state (10^{-5} cm^2 V^{-1} s^{-1}; R_E = ratio of potential gradients; t = time-based zone length of a 10-nmol sample (s); R_S = specific resistance of the separated zones (Ω m); IS = ionic strength of the separated zones (mM).

400	$C_6H_{12}N_2O_3$		Ala-Ala					-27.0		8.490	160.2	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.89	7.92	7.97	8.03	8.10	8.19	8.38	8.42	8.49	8.57	8.67	8.79
mS	5.32	5.64	6.11	6.76	7.62	8.74	11.31	11.95	12.82	13.96	15.33	16.86
RE	14.04	13.24	12.23	11.06	9.80	8.55	6.60	6.25	5.82	5.35	4.87	4.43
t	28.65	28.66	28.68	28.70	28.73	28.76	20.32	20.32	20.33	20.34	20.36	20.39
RS	118.5	111.7	103.2	93.28	82.65	72.11	67.88	64.26	59.87	54.99	50.06	45.51
IS	1.14	1.21	1.32	1.46	1.65	1.90	2.89	3.06	3.29	3.59	3.96	4.37

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.81	8.89	9.00	9.13	9.28	9.45	9.39	9.53	9.70	9.89	10.08	10.29
mS	17.13	18.03	19.10	20.23	21.30	22.20	21.97	22.62	23.18	23.61	23.93	24.16
RE	4.36	4.14	3.91	3.69	3.51	3.36	3.40	3.30	3.22	3.16	3.12	3.09
t	21.36	21.38	21.41	21.47	21.56	21.70	26.45	26.63	26.91	27.39	28.22	29.69
RS	43.74	41.55	39.22	37.00	35.12	33.65	30.50	29.58	28.81	28.20	27.70	27.23
IS	4.34	4.57	4.85	5.14	5.42	5.63	5.07	5.21	5.31	5.36	5.35	5.24

401	$C_9H_{17}N_3O_4$		Ala-Ala-Ala					-22.2		8.245	231.3	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.78	7.82	7.87	7.94	8.02	8.12	8.28	8.33	8.41	8.51	8.63	8.77
mS	5.50	5.86	6.38	7.07	7.98	9.09	10.86	11.49	12.31	13.32	14.45	15.60
RE	13.57	12.74	11.71	10.56	9.36	8.21	6.88	6.50	6.07	5.61	5.17	4.79
t	32.97	32.99	33.02	33.06	33.12	33.18	22.79	22.80	22.82	22.84	22.88	22.92
RS	114.5	107.4	98.81	89.08	78.98	69.28	70.69	66.85	62.38	57.65	53.13	49.21
IS	1.26	1.35	1.47	1.63	1.85	2.11	3.06	3.24	3.48	3.78	4.11	4.45

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.75	8.85	8.98	9.13	9.30	9.48	9.40	9.56	9.75	9.95	10.16	10.38
mS	15.46	16.19	16.97	17.71	18.32	18.79	18.69	19.06	19.34	19.55	19.71	19.84
RE	4.83	4.61	4.40	4.22	4.08	3.97	4.00	3.92	3.86	3.82	3.79	3.76
t	24.10	24.14	24.20	24.29	24.44	24.66	30.48	30.78	31.27	32.12	33.63	36.60
RS	48.48	46.29	44.14	42.28	40.82	39.75	35.84	35.11	34.53	34.06	33.63	33.15
IS	4.28	4.49	4.71	4.92	5.08	5.18	4.62	4.69	4.71	4.68	4.58	4.37

402	$C_7H_{14}N_2O_3$		Ala-Amin					-25.8		8.495	174.2	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.89	7.93	7.97	8.03	8.11	8.20	8.38	8.43	8.49	8.57	8.68	8.80
mS	5.07	5.38	5.84	6.46	7.30	8.38	10.78	11.39	12.24	13.33	14.65	16.11
RE	14.74	13.88	12.80	11.55	10.23	8.91	6.93	6.56	6.10	5.60	5.10	4.64
t	29.57	29.58	29.60	29.62	29.66	29.70	20.85	20.86	20.87	20.88	20.90	20.93
RS	124.3	117.0	108.0	97.47	86.26	75.19	71.24	67.39	62.73	57.58	52.40	47.63
IS	1.11	1.18	1.28	1.42	1.60	1.85	2.81	2.98	3.21	3.51	3.87	4.27

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.82	8.90	9.01	9.14	9.29	9.46	9.40	9.55	9.72	9.90	10.10	10.31
mS	16.34	17.21	18.23	19.32	20.33	21.18	20.97	21.59	22.12	22.53	22.83	23.05
RE	4.57	4.34	4.10	3.87	3.67	3.53	3.56	3.46	3.38	3.32	3.27	3.24
t	21.95	21.97	22.01	22.08	22.18	22.33	27.32	27.52	27.84	28.39	29.33	31.04
RS	45.86	43.54	41.08	38.76	36.79	35.27	31.95	30.99	30.19	29.56	29.03	28.54
IS	4.22	4.45	4.73	5.01	5.27	5.48	4.92	5.05	5.15	5.19	5.16	5.03

403	$C_7H_{13}N_3O_4$		Ala-Asn					-25.5		8.470	203.2	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.88	7.92	7.96	8.02	8.10	8.19	8.37	8.42	8.48	8.57	8.67	8.80
mS	5.13	5.45	5.91	6.55	7.40	8.48	10.83	11.45	12.30	13.39	14.70	16.14
RE	14.56	13.71	12.64	11.41	10.10	8.81	6.90	6.52	6.07	5.58	5.08	4.63
t	29.81	29.82	29.84	29.87	29.90	29.95	20.99	21.00	21.01	21.02	21.04	21.07
RS	122.8	115.6	106.6	96.25	85.19	74.30	70.88	67.04	62.42	57.33	52.23	47.56
IS	1.12	1.20	1.30	1.44	1.63	1.88	2.85	3.01	3.25	3.54	3.90	4.30

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.81	8.89	9.00	9.14	9.29	9.47	9.40	9.55	9.72	9.91	10.11	10.32
mS	16.32	17.18	18.19	19.24	20.21	21.02	20.82	21.41	21.91	22.30	22.58	22.79
RE	4.58	4.35	4.11	3.88	3.70	3.55	3.59	3.49	3.41	3.35	3.31	3.28
t	22.10	22.13	22.17	22.23	22.34	22.50	27.54	27.75	28.08	28.65	29.62	31.41
RS	45.92	43.61	41.19	38.92	37.01	35.54	32.18	31.25	30.48	29.86	29.35	28.86
IS	4.24	4.47	4.74	5.02	5.27	5.47	4.91	5.03	5.12	5.15	5.11	4.98

404	$C_5H_{10}N_2O_3$			Ala-Gly				-28.8		8.390	146.1	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.84	7.87	7.91	7.97	8.05	8.14	8.33	8.38	8.44	8.52	8.63	8.75
mS	6.20	6.57	7.09	7.82	8.80	10.05	12.88	13.58	14.53	15.76	17.23	18.84
RE	12.04	11.37	10.53	9.55	8.49	7.44	5.80	5.50	5.14	4.74	4.34	3.97
t	27.42	27.43	27.45	27.47	27.49	27.52	19.60	19.60	19.61	19.62	19.63	19.65
RS	101.6	95.94	88.85	80.56	71.61	62.72	59.63	56.55	52.83	48.70	44.55	40.74
IS	1.31	1.38	1.50	1.65	1.87	2.14	3.19	3.37	3.62	3.94	4.32	4.74

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.77	8.85	8.96	9.10	9.25	9.43	9.35	9.50	9.67	9.86	10.06	10.27
mS	19.03	19.97	21.07	22.21	23.25	24.10	23.85	24.48	25.00	25.40	25.69	25.90
RE	3.93	3.74	3.55	3.36	3.21	3.10	3.13	3.05	2.99	2.94	2.91	2.88
t	20.55	20.57	20.60	20.65	20.72	20.84	25.28	25.42	25.67	26.07	26.75	27.95
RS	39.39	37.52	35.55	33.71	32.18	30.99	28.09	27.34	26.71	26.21	25.80	25.40
IS	4.68	4.92	5.20	5.49	5.75	5.95	5.39	5.52	5.61	5.66	5.65	5.56

405	$C_7H_{13}N_3O_4$			Ala-Gly-Gly				-25.0		8.254	203.2	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.78	7.81	7.86	7.93	8.01	8.10	8.28	8.33	8.40	8.49	8.61	8.75
mS	6.11	6.50	7.04	7.78	8.76	9.97	12.16	12.83	13.73	14.85	16.12	17.44
RE	12.22	11.50	10.61	9.60	8.53	7.49	6.14	5.82	5.44	5.03	4.63	4.28
t	30.25	30.27	30.29	30.32	30.36	30.40	21.22	21.22	21.23	21.25	21.27	21.30
RS	103.0	97.00	89.54	80.98	71.96	63.18	63.14	59.83	55.91	51.70	47.61	44.00
IS	1.35	1.44	1.56	1.73	1.95	2.23	3.24	3.43	3.68	3.99	4.35	4.71

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.73	8.83	8.95	9.10	9.27	9.45	9.36	9.53	9.71	9.90	10.11	10.32
mS	17.36	18.17	19.06	19.93	20.66	21.23	21.07	21.51	21.85	22.11	22.29	22.43
RE	4.30	4.11	3.92	3.75	3.62	3.52	3.54	3.47	3.42	3.38	3.35	3.33
t	22.35	22.37	22.42	22.48	22.59	22.76	27.89	28.11	28.46	29.06	30.09	31.99
RS	43.18	41.24	39.29	37.57	36.20	35.19	31.79	31.11	30.56	30.12	29.73	29.32
IS	4.57	4.79	5.04	5.26	5.45	5.59	5.01	5.10	5.15	5.14	5.08	4.92

406	$C_9H_{14}N_4O_3$			β-Ala-His				-24.4		9.664	226.2	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.78	7.81	7.86	7.93	8.01	8.74	8.95	8.99	9.03	9.09	9.16	9.25
mS	0.00	0.00	0.00	0.00	0.00	2.57	3.91	4.16	4.51	5.01	5.69	6.56
RE	0.00	0.00	0.00	0.00	0.00	29.10	19.10	17.96	16.55	14.90	13.14	11.39
t	0.00	0.00	0.00	0.00	0.00	31.59	22.27	22.29	22.31	22.34	22.38	22.45
RS	0.00	0.00	0.00	0.00	0.00	245.5	196.3	184.7	170.1	153.1	135.0	117.0
IS	0.00	0.00	0.00	0.00	0.00	0.55	0.99	1.06	1.15	1.28	1.45	1.68

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	9.34	9.39	9.45	9.53	9.63	9.74	9.80	9.88	9.98	10.11	10.26	10.43
mS	7.65	8.19	8.94	9.91	11.14	12.57	13.38	14.29	15.41	16.68	17.97	19.19
RE	9.76	9.12	8.36	7.53	6.71	5.94	5.58	5.23	4.85	4.48	4.16	3.89
t	23.62	23.67	23.75	23.86	24.03	24.29	29.97	30.27	30.75	31.54	32.92	35.51
RS	97.91	91.46	83.83	75.51	67.18	59.45	50.09	46.83	43.34	39.93	36.87	34.27
IS	1.91	2.05	2.24	2.48	2.79	3.14	3.02	3.22	3.45	3.68	3.88	3.97

407	$C_9H_{18}N_2O_3$			Ala-Leu				-23.9		8.505	202.3	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.90	7.94	7.98	8.04	8.12	8.21	8.39	8.44	8.50	8.59	8.69	8.82
mS	4.67	4.97	5.40	6.00	6.79	7.80	9.93	10.51	11.31	12.33	13.56	14.92
RE	16.00	15.03	13.83	12.45	11.00	9.57	7.53	7.11	6.61	6.06	5.51	5.01
t	31.21	31.23	31.25	31.28	31.32	31.37	21.81	21.81	21.83	21.85	21.87	21.91
RS	134.9	126.8	116.7	105.1	92.78	80.76	77.36	73.06	67.91	62.26	56.61	51.45
IS	1.04	1.11	1.21	1.35	1.53	1.76	2.68	2.85	3.07	3.36	3.71	4.09

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.83	8.91	9.02	9.16	9.31	9.48	9.42	9.57	9.74	9.93	10.13	10.35
mS	15.08	15.90	16.86	17.86	18.79	19.57	19.39	19.96	20.44	20.81	21.09	21.30
RE	4.95	4.70	4.43	4.18	3.98	3.82	3.85	3.74	3.65	3.59	3.54	3.51
t	23.02	23.05	23.10	23.18	23.30	23.49	28.89	29.14	29.54	30.22	31.41	33.66
RS	49.69	47.12	44.44	41.92	39.81	38.18	34.55	33.52	32.67	31.99	31.43	30.88
IS	4.03	4.25	4.52	4.79	5.03	5.23	4.67	4.79	4.87	4.89	4.84	4.68

408	$C_{11}H_{21}N_3O_4$			Ala-Leu-Gly				-21.3		8.272	259.3	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.79	7.83	7.89	7.95	8.04	8.14	8.29	8.35	8.43	8.52	8.64	8.78
mS	5.17	5.51	6.00	6.67	7.54	8.60	10.26	10.86	11.65	12.63	13.72	14.83
RE	14.46	13.55	12.44	11.20	9.91	8.68	7.28	6.88	6.41	5.92	5.45	5.04
t	33.99	34.02	34.05	34.10	34.16	34.23	23.39	23.41	23.43	23.45	23.49	23.54
RS	121.9	114.3	104.9	94.44	83.60	73.24	74.83	70.69	65.88	60.81	55.96	51.75
IS	1.20	1.28	1.40	1.56	1.76	2.02	2.94	3.12	3.35	3.64	3.97	4.30

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.76	8.86	8.99	9.14	9.31	9.50	9.41	9.58	9.77	9.97	10.18	10.40
mS	14.70	15.41	16.17	16.89	17.49	17.96	17.87	18.22	18.50	18.71	18.86	19.01
RE	5.08	4.85	4.62	4.42	4.27	4.16	4.18	4.10	4.04	3.99	3.96	3.93
t	24.78	24.82	24.89	24.99	25.15	25.40	31.48	31.82	32.38	33.34	35.08	38.61
RS	50.99	48.64	46.33	44.33	42.77	41.61	37.50	36.72	36.10	35.59	35.13	34.60
IS	4.14	4.34	4.56	4.76	4.92	5.03	4.47	4.53	4.55	4.51	4.40	4.16

409	$C_8H_{16}N_2O_3S$			Ala-Met				-24.2		8.463	220.3	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.88	7.91	7.96	8.02	8.10	8.19	8.37	8.42	8.48	8.57	8.68	8.80
mS	4.91	5.23	5.68	6.30	7.12	8.17	10.33	10.93	11.75	12.80	14.05	15.41
RE	15.21	14.29	13.16	11.86	10.49	9.14	7.23	6.83	6.36	5.84	5.32	4.85
t	30.94	30.95	30.98	31.01	31.05	31.09	21.64	21.65	21.66	21.68	21.71	21.74
RS	128.3	120.6	111.0	100.1	88.46	77.11	74.31	70.22	65.33	59.98	54.65	49.80
IS	1.10	1.17	1.27	1.41	1.60	1.84	2.78	2.95	3.18	3.47	3.82	4.21

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.81	8.90	9.01	9.15	9.30	9.48	9.41	9.56	9.73	9.92	10.13	10.34
mS	15.54	16.36	17.32	18.30	19.21	19.96	19.78	20.33	20.79	21.14	21.40	21.60
RE	4.81	4.57	4.31	4.08	3.89	3.74	3.78	3.67	3.59	3.53	3.49	3.46
t	22.83	22.86	22.91	22.98	23.10	23.28	28.62	28.85	29.24	29.89	31.04	33.18
RS	48.23	45.79	43.26	40.90	38.94	37.44	33.87	32.92	32.13	31.50	30.97	30.46
IS	4.13	4.36	4.62	4.89	5.12	5.31	4.74	4.86	4.93	4.95	4.90	4.74

410	$C_3H_7NO_2$			β-Alanine				36.7 -30.8		3.552 10.241	89.1	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.88	7.91	7.96	8.02	8.10	8.19	9.25	9.28	9.31	9.36	9.42	9.50
mS	0.00	0.00	0.00	0.00	0.00	0.00	2.84	3.00	3.24	3.58	4.05	4.68
RE	0.00	0.00	0.00	0.00	0.00	0.00	26.35	24.92	23.09	20.89	18.45	15.95
t	0.00	0.00	0.00	0.00	0.00	0.00	21.15	21.16	21.19	21.22	21.26	21.33
RS	0.00	0.00	0.00	0.00	0.00	0.00	270.8	256.2	237.3	214.7	189.6	163.9
IS	0.00	0.00	0.00	0.00	0.00	0.00	0.60	0.64	0.69	0.76	0.86	1.00

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	9.63	9.66	9.71	9.78	9.85	9.94	10.06	10.11	10.18	10.27	10.38	10.51
mS	5.99	6.38	6.95	7.73	8.77	10.11	11.84	12.68	13.81	15.28	17.05	19.07
RE	12.48	11.71	10.76	9.67	8.52	7.39	6.31	5.89	5.41	4.89	4.38	3.92
t	22.37	22.42	22.50	22.61	22.78	23.04	27.95	28.21	28.63	29.28	30.34	32.18
RS	125.2	117.4	107.9	96.87	85.28	73.92	56.59	52.79	48.35	43.59	38.86	34.49
IS	1.25	1.34	1.45	1.62	1.83	2.10	2.29	2.44	2.65	2.90	3.19	3.46

411	$C_3H_7NO_2$			Alanine				-32.7		9.862	89.1	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.88	7.91	7.96	8.02	8.10	8.80	9.04	9.07	9.11	9.16	9.23	9.30
mS	0.00	0.00	0.00	0.00	0.00	2.61	4.27	4.51	4.87	5.38	6.07	7.00
RE	0.00	0.00	0.00	0.00	0.00	28.59	17.51	16.56	15.34	13.89	12.30	10.67
t	0.00	0.00	0.00	0.00	0.00	26.09	19.17	19.18	19.19	19.20	19.23	19.26
RS	0.00	0.00	0.00	0.00	0.00	241.2	180.0	170.2	157.7	142.8	126.4	109.6
IS	0.00	0.00	0.00	0.00	0.00	0.51	0.93	0.98	1.06	1.17	1.33	1.54

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	9.42	9.46	9.51	9.58	9.67	9.77	9.85	9.91	9.99	10.10	10.22	10.37
mS	8.58	9.14	9.94	11.02	12.41	14.13	15.59	16.65	18.03	19.70	21.57	23.49
RE	8.70	8.17	7.52	6.78	6.02	5.28	4.79	4.49	4.14	3.79	3.46	3.18
t	20.12	20.15	20.19	20.25	20.35	20.49	24.66	24.81	25.05	25.43	26.04	27.08
RS	87.30	81.93	75.37	67.97	60.27	52.86	42.96	40.19	37.05	33.80	30.72	28.00
IS	1.86	1.98	2.15	2.39	2.69	3.07	3.15	3.36	3.63	3.95	4.28	4.59

412	$C_{12}H_{16}N_2O_3$			Ala-Phe				-23.9		8.502	236.3	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.90	7.93	7.98	8.04	8.12	8.21	8.39	8.44	8.50	8.59	8.69	8.81
mS	4.68	4.98	5.42	6.01	6.81	7.82	9.95	10.53	11.33	12.35	13.58	14.94
RE	15.95	14.99	13.79	12.42	10.97	9.55	7.51	7.09	6.59	6.05	5.50	5.00
t	31.21	31.23	31.25	31.28	31.32	31.37	21.81	21.81	21.83	21.85	21.87	21.91
RS	134.6	126.4	116.3	104.8	92.54	80.56	77.21	72.92	67.78	62.14	56.51	51.38
IS	1.05	1.12	1.21	1.35	1.53	1.77	2.69	2.85	3.08	3.37	3.71	4.10

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.83	8.91	9.02	9.16	9.31	9.48	9.42	9.57	9.74	9.93	10.13	10.35
mS	15.10	15.92	16.87	17.87	18.80	19.58	19.40	19.97	20.45	20.82	21.09	21.30
RE	4.95	4.69	4.43	4.18	3.97	3.82	3.85	3.74	3.65	3.59	3.54	3.51
t	23.02	23.05	23.10	23.18	23.30	23.49	28.89	29.14	29.54	30.22	31.41	33.66
RS	49.62	47.07	44.39	41.89	39.79	38.16	34.53	33.51	32.66	31.99	31.43	30.88
IS	4.04	4.26	4.52	4.79	5.04	5.23	4.67	4.79	4.87	4.89	4.84	4.68

413	$C_6H_{12}O_4N_2$			Ala-Ser				-26.2		8.297	176.2	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.80	7.83	7.88	7.94	8.02	8.11	8.29	8.34	8.41	8.50	8.61	8.75
mS	6.16	6.53	7.07	7.81	8.79	10.02	12.42	13.10	14.02	15.18	16.52	17.93
RE	12.13	11.43	10.56	9.56	8.50	7.45	6.02	5.70	5.33	4.92	4.52	4.17
t	29.27	29.28	29.30	29.32	29.36	29.40	20.65	20.66	20.67	20.68	20.70	20.72
RS	102.3	96.43	89.11	80.65	71.67	62.87	61.83	58.60	54.76	50.58	46.47	42.80
IS	1.34	1.43	1.55	1.71	1.93	2.21	3.24	3.42	3.67	3.98	4.35	4.74

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.74	8.84	8.96	9.10	9.26	9.44	9.36	9.52	9.70	9.89	10.09	10.30
mS	17.92	18.78	19.74	20.69	21.51	22.17	21.98	22.47	22.87	23.16	23.37	23.53
RE	4.17	3.98	3.78	3.61	3.47	3.37	3.40	3.32	3.27	3.22	3.20	3.17
t	21.72	21.74	21.78	21.84	21.93	22.08	26.98	27.16	27.48	28.00	28.89	30.52
RS	41.82	39.90	37.95	36.19	34.77	33.70	30.49	29.78	29.21	28.75	28.36	27.95
IS	4.62	4.85	5.10	5.35	5.56	5.71	5.14	5.24	5.31	5.32	5.27	5.14

414	$C_8H_{16}N_2O_3$			Ala-Val				-25.2		8.500	188.2	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.90	7.93	7.98	8.04	8.11	8.20	8.39	8.43	8.50	8.58	8.68	8.81
mS	4.93	5.24	5.69	6.31	7.13	8.18	10.49	11.10	11.93	13.00	14.29	15.72
RE	15.14	14.25	13.13	11.85	10.48	9.13	7.12	6.73	6.26	5.75	5.23	4.75
t	30.06	30.07	30.09	30.12	30.15	30.20	21.14	21.14	21.15	21.17	21.19	21.22
RS	127.7	120.2	110.8	99.92	88.37	77.00	73.17	69.17	64.36	59.05	53.72	48.82
IS	1.09	1.15	1.25	1.39	1.58	1.82	2.77	2.93	3.16	3.46	3.81	4.21

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.82	8.90	9.01	9.14	9.30	9.47	9.41	9.55	9.72	9.91	10.11	10.32
mS	15.93	16.78	17.79	18.84	19.83	20.66	20.47	21.07	21.58	21.98	22.27	22.49
RE	4.69	4.45	4.20	3.96	3.77	3.61	3.65	3.54	3.46	3.40	3.35	3.32
t	22.27	22.30	22.34	22.41	22.51	22.68	27.79	28.00	28.35	28.93	29.94	31.80
RS	47.04	44.65	42.11	39.73	37.71	36.16	32.74	31.76	30.94	30.29	29.75	29.24
IS	4.16	4.39	4.66	4.94	5.20	5.40	4.84	4.97	5.06	5.09	5.06	4.92

415	$C_5H_{11}O_2N$			α-Amino-n-butyric acid				-30.5		9.827	117.1	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.90	7.93	7.98	8.04	8.11	8.79	9.03	9.06	9.10	9.15	9.21	9.29
mS	0.00	0.00	0.00	0.00	0.00	2.57	4.13	4.38	4.73	5.23	5.91	6.82
RE	0.00	0.00	0.00	0.00	0.00	29.09	18.07	17.07	15.80	14.29	12.63	10.95
t	0.00	0.00	0.00	0.00	0.00	27.27	19.84	19.85	19.86	19.88	19.91	19.95
RS	0.00	0.00	0.00	0.00	0.00	245.4	185.8	175.5	162.4	146.8	129.8	112.5
IS	0.00	0.00	0.00	0.00	0.00	0.51	0.93	0.99	1.07	1.19	1.34	1.55

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	9.41	9.45	9.50	9.57	9.66	9.76	9.84	9.91	9.99	10.10	10.23	10.38
mS	8.28	8.83	9.61	10.65	12.00	13.65	14.95	15.97	17.29	18.86	20.60	22.36
RE	9.02	8.46	7.78	7.01	6.22	5.47	5.00	4.68	4.32	3.96	3.62	3.34
t	20.88	20.91	20.96	21.03	21.14	21.30	25.80	25.98	26.26	26.71	27.45	28.72
RS	90.51	84.85	77.98	70.27	62.32	54.73	44.81	41.90	38.64	35.30	32.16	29.42
IS	1.85	1.98	2.16	2.39	2.70	3.07	3.10	3.31	3.57	3.88	4.19	4.45

416	$C_6H_{14}N_4O_2$				Arginine							
417	$C_4H_8N_2O_3$				Asparagine				-32.1		9.051	132.1
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	8.16	8.19	8.22	8.27	8.34	8.41	8.64	8.67	8.72	8.78	8.86	8.95
mS	3.62	3.83	4.13	4.56	5.16	5.95	8.77	9.27	9.97	10.95	12.23	13.83
RE	20.61	19.50	18.08	16.37	14.49	12.55	8.52	8.06	7.49	6.82	6.11	5.40
t	25.59	25.60	25.61	25.62	25.63	25.65	18.64	18.64	18.64	18.65	18.66	18.68
RS	173.8	164.5	152.5	138.1	122.2	105.9	87.55	82.87	76.98	70.12	62.75	55.49
IS	0.72	0.77	0.83	0.91	1.04	1.20	2.02	2.13	2.30	2.53	2.84	3.22

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	9.04	9.09	9.16	9.26	9.37	9.51	9.51	9.61	9.74	9.89	10.06	10.25
mS	15.20	16.11	17.32	18.83	20.56	22.35	22.47	23.60	24.83	26.01	27.02	27.81
RE	4.92	4.64	4.31	3.97	3.63	3.34	3.32	3.17	3.01	2.87	2.76	2.69
t	19.50	19.51	19.54	19.58	19.64	19.74	23.75	23.86	24.05	24.36	24.87	25.77
RS	49.31	46.51	43.24	39.76	36.39	33.43	29.82	28.36	26.90	25.60	24.53	23.65
IS	3.48	3.70	3.98	4.34	4.74	5.16	4.80	5.04	5.29	5.52	5.68	5.76

418	$C_4H_7NO_4$				Aspartic Acid			-30.1 -56.8		3.900 10.017	133.1	
No.	1	2	3	4	5	6	7	8	9	10	11	12
pHL	2.60	2.80	3.00	3.20	3.40	3.60	3.00	3.20	3.40	3.60	3.80	4.00
pHS	3.56	3.65	3.74	3.83	3.93	4.04	3.74	3.83	3.92	4.03	4.16	4.30
mS	8.48	9.99	11.48	13.01	14.66	16.45	11.44	12.95	14.57	16.34	18.20	20.06
RE	8.81	7.47	6.50	5.74	5.10	4.54	6.53	5.77	5.13	4.57	4.10	3.72
t	35.45	30.27	26.89	24.42	22.55	21.16	25.77	23.32	21.45	20.05	19.06	18.39
RS	50.44	51.42	51.30	49.87	47.30	44.07	52.66	51.41	48.94	45.70	42.28	39.12
IS	2.09	2.36	2.63	2.97	3.38	3.87	2.68	3.02	3.44	3.94	4.49	5.05

No.	13	14	15	16	17	18	19	20	21	22	23	24
pHL	3.80	4.00	4.20	4.40	4.60	4.80	4.20	4.40	4.60	4.80	5.00	5.20
pHS	4.32	4.42	4.53	4.67	4.82	5.00	4.62	4.73	4.87	5.03	5.21	5.40
mS	20.41	21.48	22.59	23.68	24.66	25.46	23.38	24.20	24.98	25.67	26.20	26.58
RE	3.66	3.48	3.31	3.15	3.03	2.93	3.19	3.09	2.99	2.91	2.85	2.81
t	19.96	19.70	19.47	19.28	19.13	19.03	22.25	22.12	22.01	21.93	21.87	21.83
RS	36.01	34.86	33.54	32.23	31.09	30.21	29.99	29.18	28.39	27.71	27.19	26.83
IS	5.05	5.29	5.57	5.87	6.14	6.36	5.45	5.64	5.83	6.01	6.14	6.24

No.	25	26	27	28	29	30	31
pHL	5.40	5.40	5.60	5.80	6.00	6.20	6.40
pHS	5.59	5.59	5.78	5.97	6.16	6.36	6.56
mS	26.84	26.77	26.93	27.05	27.12	27.17	27.20
RE	2.78	2.79	2.77	2.76	2.75	2.75	2.75
t	21.81	19.17	19.16	19.15	19.14	19.14	19.14
RS	26.58	28.61	28.46	28.35	28.28	28.23	28.20
IS	6.31	6.69	6.73	6.76	6.78	6.80	6.81

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	6.62	6.82	7.02	7.22	7.42	7.62	7.57	7.77	7.97	8.17	8.37	8.57
mS	27.39	27.41	27.43	27.46	27.49	27.53	27.34	27.40	27.49	27.63	27.85	28.20
RE	2.73	2.72	2.72	2.72	2.72	2.71	2.73	2.73	2.72	2.70	2.68	2.65
t	26.89	26.90	26.91	26.92	26.95	26.99	19.18	19.23	19.32	19.45	19.65	19.95
RS	23.00	22.99	22.97	22.95	22.92	22.89	28.09	28.02	27.93	27.78	27.56	27.22
IS	5.90	5.90	5.91	5.92	5.93	5.94	6.85	6.87	6.90	6.94	7.01	7.11

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.40	8.60	8.79	8.99	9.18	9.37	9.28	9.45	9.62	9.79	9.97	10.15
mS	27.93	28.29	28.84	29.63	30.75	32.25	31.58	33.08	34.87	36.91	39.06	41.18
RE	2.67	2.64	2.59	2.52	2.43	2.32	2.37	2.26	2.14	2.02	1.91	1.81
t	20.56	20.89	21.36	22.02	22.91	24.02	27.87	29.03	30.30	31.67	33.07	34.59
RS	26.84	26.49	25.98	25.26	24.32	23.17	21.21	20.23	19.15	18.04	16.96	15.97
IS	6.89	7.00	7.16	7.40	7.74	8.18	7.46	7.90	8.43	9.03	9.66	10.25

419	$C_3H_7NO_2S$			Cysteine					-31.7 -62.7	8.600 10.280	121.2	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.94	7.97	8.01	8.06	8.13	8.21	8.42	8.46	8.52	8.59	8.69	8.80
mS	5.64	5.96	6.43	7.09	7.99	9.18	12.61	13.32	14.31	15.65	17.36	19.39
RE	13.24	12.53	11.61	10.53	9.34	8.14	5.92	5.61	5.22	4.77	4.30	3.85
t	25.84	25.86	25.88	25.90	25.94	26.00	18.97	19.00	19.05	19.13	19.24	19.42
RS	111.7	105.7	97.97	88.84	78.82	68.66	60.88	57.65	53.64	49.05	44.23	39.58
IS	1.14	1.21	1.31	1.45	1.63	1.88	2.96	3.14	3.38	3.71	4.12	4.63

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.85	8.92	9.01	9.13	9.27	9.43	9.40	9.52	9.67	9.82	9.99	10.16
mS	20.30	21.52	23.10	25.00	27.17	29.53	29.26	31.08	33.25	35.75	38.48	41.31
RE	3.68	3.47	3.23	2.99	2.75	2.53	2.55	2.40	2.25	2.09	1.94	1.81
t	20.33	20.48	20.71	21.06	21.59	22.33	26.31	27.00	27.92	29.11	30.46	31.94
RS	36.91	34.82	32.43	29.94	27.53	25.30	22.90	21.53	20.08	18.63	17.22	15.92
IS	4.77	5.07	5.45	5.93	6.47	7.06	6.56	7.02	7.57	8.20	8.90	9.63

420	$C_6H_{12}N_2O_4S_2$			Cystine					-27.0 -53.9	8.405 9.845	240.3	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.85	7.88	7.93	7.98	8.06	8.15	8.34	8.39	8.45	8.53	8.64	8.76
mS	5.86	6.22	6.74	7.46	8.43	9.69	12.63	13.38	14.43	15.81	17.53	19.55
RE	12.75	12.01	11.09	10.01	8.86	7.71	5.91	5.58	5.18	4.73	4.26	3.82
t	28.87	28.90	28.95	29.01	29.09	29.21	20.99	21.07	21.19	21.38	21.65	22.04
RS	107.5	101.3	93.51	84.44	74.71	65.05	60.79	57.37	53.21	48.56	43.79	39.25
IS	1.27	1.35	1.46	1.62	1.84	2.12	3.25	3.45	3.73	4.11	4.58	5.14

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.79	8.87	8.98	9.11	9.26	9.42	9.38	9.51	9.65	9.81	9.97	10.15
mS	20.04	21.34	23.02	25.02	27.31	29.81	29.38	31.32	33.51	35.80	38.05	40.06
RE	3.73	3.50	3.25	2.99	2.74	2.51	2.54	2.39	2.23	2.09	1.96	1.86
t	23.12	23.45	23.92	24.60	25.47	26.53	31.22	32.09	33.11	34.18	35.37	36.67
RS	37.40	35.10	32.54	29.92	27.39	25.06	22.80	21.37	19.93	18.60	17.42	16.42
IS	5.17	5.53	5.99	6.56	7.22	7.93	7.30	7.86	8.49	9.16	9.80	10.35

421	$C_5H_9NO_4$			Glutamic Acid					-26.8 -55.7	4.324 9.966	147.1	
No.	1	2	3	4	5	6	7	8	9	10	11	12
pHL	2.60	2.80	3.00	3.20	3.40	3.60	3.00	3.20	3.40	3.60	3.80	4.00
pHS	3.77	3.86	3.94	4.02	4.11	4.20	3.94	4.02	4.10	4.20	4.31	4.43
mS	5.19	6.20	7.23	8.31	9.53	10.93	7.20	8.26	9.46	10.84	12.40	14.12
RE	14.40	12.04	10.33	8.99	7.84	6.83	10.38	9.04	7.90	6.89	6.02	5.29
t	38.32	32.67	29.00	26.31	24.25	22.72	27.74	25.07	23.02	21.47	20.36	19.61
RS	82.44	82.84	81.51	78.07	72.77	66.32	83.73	80.58	75.40	68.92	62.05	55.59
IS	1.36	1.55	1.74	1.99	2.30	2.69	1.78	2.02	2.34	2.74	3.22	3.74

No.	13	14	15	16	17	18	19	20	21	22	23	24
pHL	3.80	4.00	4.20	4.40	4.60	4.80	4.20	4.40	4.60	4.80	5.00	5.20
pHS	4.49	4.57	4.66	4.78	4.91	5.07	4.77	4.86	4.97	5.11	5.27	5.45
mS	15.02	16.02	17.14	18.37	19.63	20.78	18.32	19.21	20.18	21.14	22.00	22.68
RE	4.97	4.66	4.36	4.07	3.81	3.59	4.08	3.89	3.70	3.53	3.40	3.29
t	21.19	20.95	20.73	20.54	20.40	20.29	23.84	23.73	23.63	23.55	23.49	23.45
RS	48.94	46.74	44.20	41.55	39.07	37.01	38.28	36.75	35.14	33.63	32.38	31.45
IS	3.93	4.17	4.46	4.80	5.16	5.49	4.48	4.70	4.94	5.19	5.41	5.59

No.	25	26	27	28	29	30	31
pHL	5.40	5.40	5.60	5.80	6.00	6.20	6.40
pHS	5.64	5.66	5.82	6.00	6.20	6.39	6.59
mS	23.17	23.15	23.44	23.66	23.81	23.91	23.98
RE	3.22	3.23	3.19	3.16	3.14	3.12	3.11
t	23.43	20.45	20.44	20.42	20.42	20.42	20.42
RS	30.79	33.09	32.70	32.41	32.21	32.07	31.99
IS	5.72	6.12	6.21	6.27	6.31	6.34	6.36

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	6.66	6.86	7.06	7.26	7.45	7.65	7.60	7.79	7.99	8.19	8.39	8.59
mS	24.19	24.23	24.27	24.31	24.35	24.41	24.20	24.28	24.40	24.59	24.88	25.32
RE	3.09	3.08	3.08	3.07	3.07	3.06	3.09	3.08	3.06	3.04	3.00	2.95
t	29.18	29.18	29.19	29.21	29.24	29.29	20.47	20.54	20.63	20.79	21.02	21.37
RS	26.05	26.00	25.96	25.92	25.88	25.81	31.73	31.62	31.46	31.22	30.85	30.31
IS	5.42	5.43	5.44	5.45	5.47	5.48	6.43	6.45	6.48	6.54	6.61	6.74

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.44	8.63	8.83	9.02	9.21	9.39	9.32	9.48	9.64	9.81	9.98	10.16
mS	24.99	25.46	26.16	27.16	28.53	30.31	29.65	31.36	33.36	35.59	37.89	40.12
RE	2.99	2.93	2.86	2.75	2.62	2.46	2.52	2.38	2.24	2.10	1.97	1.86
t	22.07	22.44	22.96	23.68	24.58	25.67	30.05	31.08	32.18	33.34	34.52	35.83
RS	29.99	29.43	28.63	27.56	26.22	24.65	22.59	21.34	20.02	18.71	17.49	16.40
IS	6.49	6.63	6.82	7.10	7.48	7.97	7.26	7.73	8.29	8.92	9.56	10.16

422 $C_5H_{10}N_2O_3$ Glutamine -30.1 9.308 146.1

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	8.29	8.32	8.35	8.40	8.47	8.54	8.76	8.80	8.84	8.90	8.98	9.07
mS	2.62	2.77	3.00	3.32	3.76	4.36	6.59	6.98	7.54	8.31	9.34	10.66
RE	28.54	26.96	24.94	22.52	19.86	17.14	11.33	10.70	9.91	8.99	8.00	7.01
t	26.79	26.80	26.81	26.82	26.84	26.87	19.39	19.39	19.40	19.41	19.43	19.45
RS	240.7	227.4	210.3	190.0	167.5	144.6	116.4	110.0	101.9	92.40	82.18	72.02
IS	0.53	0.56	0.61	0.68	0.77	0.89	1.55	1.64	1.78	1.96	2.21	2.53

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	9.16	9.21	9.27	9.36	9.46	9.59	9.62	9.71	9.82	9.96	10.12	10.30
mS	12.07	12.84	13.89	15.24	16.85	18.64	19.12	20.23	21.52	22.87	24.12	25.18
RE	6.19	5.82	5.38	4.90	4.43	4.01	3.91	3.69	3.47	3.27	3.10	2.97
t	20.34	20.37	20.40	20.45	20.53	20.66	25.00	25.15	25.38	25.76	26.40	27.51
RS	62.08	58.34	53.92	49.13	44.39	40.07	35.04	33.08	31.03	29.12	27.47	26.13
IS	2.82	3.01	3.26	3.58	3.97	4.39	4.14	4.38	4.65	4.91	5.13	5.25

423 $C_5H_{10}N_2O_3$ Gly-Ala -28.8 8.435 146.1

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.86	7.89	7.94	7.99	8.07	8.16	8.35	8.40	8.46	8.54	8.64	8.77
mS	5.95	6.30	6.81	7.51	8.46	9.67	12.51	13.19	14.13	15.35	16.81	18.43
RE	12.55	11.85	10.97	9.94	8.83	7.73	5.97	5.66	5.29	4.87	4.44	4.05
t	27.42	27.43	27.45	27.46	27.49	27.52	19.61	19.61	19.61	19.62	19.63	19.65
RS	105.8	99.96	92.55	83.87	74.51	65.17	61.39	58.20	54.33	50.02	45.66	41.64
IS	1.25	1.33	1.44	1.59	1.79	2.05	3.10	3.28	3.52	3.83	4.21	4.63

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.79	8.87	8.97	9.11	9.26	9.43	9.36	9.51	9.68	9.86	10.06	10.27
mS	18.69	19.63	20.75	21.93	23.02	23.93	23.67	24.33	24.90	25.33	25.64	25.87
RE	4.00	3.80	3.60	3.41	3.24	3.12	3.16	3.07	3.00	2.95	2.91	2.89
t	20.56	20.58	20.61	20.65	20.73	20.85	25.29	25.43	25.67	26.08	26.76	27.96
RS	40.10	38.16	36.10	34.15	32.50	31.22	28.31	27.50	26.83	26.29	25.85	25.43
IS	4.59	4.84	5.12	5.41	5.69	5.90	5.34	5.48	5.59	5.64	5.63	5.55

424 $C_6H_{12}N_2O_3$ Gly-Amin -27.2 8.421 160.2

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.85	7.89	7.93	7.99	8.07	8.16	8.35	8.39	8.46	8.54	8.65	8.77
mS	5.71	6.05	6.55	7.24	8.16	9.33	11.93	12.59	13.49	14.66	16.05	17.57
RE	13.09	12.34	11.41	10.32	9.16	8.01	6.26	5.93	5.54	5.10	4.65	4.25
t	28.51	28.52	28.54	28.56	28.59	28.62	20.23	20.23	20.24	20.25	20.27	20.29
RS	110.4	104.1	96.23	87.07	77.26	67.54	64.39	60.99	56.90	52.37	47.83	43.67
IS	1.23	1.30	1.41	1.56	1.76	2.02	3.04	3.22	3.46	3.77	4.14	4.54

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.79	8.87	8.98	9.11	9.27	9.44	9.37	9.52	9.69	9.88	10.08	10.29
mS	17.75	18.65	19.71	20.80	21.80	22.63	22.40	23.01	23.52	23.90	24.19	24.39
RE	4.21	4.00	3.79	3.59	3.43	3.30	3.33	3.25	3.18	3.12	3.09	3.06
t	21.25	21.28	21.31	21.36	21.45	21.59	26.30	26.47	26.75	27.22	28.03	29.46
RS	42.22	40.16	38.01	35.99	34.31	33.01	29.91	29.08	28.40	27.85	27.40	26.97
IS	4.49	4.72	5.00	5.28	5.53	5.73	5.17	5.29	5.38	5.42	5.40	5.29

425 $C_6H_{11}N_3O_4$ Gly-Asn -27.5 8.388 189.2

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.84	7.87	7.92	7.98	8.05	8.14	8.33	8.38	8.44	8.53	8.63	8.76
mS	5.94	6.30	6.81	7.52	8.47	9.68	12.31	12.99	13.92	15.10	16.51	18.04
RE	12.56	11.85	10.96	9.93	8.82	7.72	6.07	5.75	5.37	4.95	4.52	4.14
t	28.30	28.31	28.32	28.34	28.37	28.41	20.10	20.11	20.11	20.12	20.14	20.16
RS	106.0	100.0	92.48	83.73	74.36	65.08	62.35	59.09	55.17	50.83	46.50	42.55
IS	1.27	1.35	1.46	1.62	1.83	2.09	3.13	3.31	3.55	3.86	4.24	4.64

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.77	8.86	8.97	9.11	9.26	9.44	9.36	9.51	9.69	9.88	10.08	10.28
mS	18.18	19.09	20.14	21.22	22.20	23.00	22.77	23.36	23.86	24.23	24.49	24.69
RE	4.11	3.91	3.71	3.52	3.36	3.25	3.28	3.20	3.13	3.08	3.05	3.02
t	21.11	21.13	21.17	21.22	21.30	21.44	26.09	26.26	26.53	26.99	27.77	29.15
RS	41.22	39.25	37.19	35.28	33.69	32.48	29.42	28.64	28.00	27.48	27.06	26.64
IS	4.57	4.81	5.08	5.36	5.61	5.80	5.23	5.36	5.44	5.48	5.45	5.35

426	$C_2H_5NO_2$			Glycine				-37.4		9.780	75.1	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.84	7.87	7.92	7.98	8.68	8.75	8.99	9.02	9.06	9.11	9.17	9.25
mS	0.00	0.00	0.00	0.00	2.74	3.17	5.24	5.53	5.95	6.55	7.38	8.48
RE	0.00	0.00	0.00	0.00	27.24	23.58	14.26	13.52	12.56	11.40	10.12	8.81
t	0.00	0.00	0.00	0.00	23.77	23.79	17.77	17.78	17.78	17.79	17.81	17.83
RS	0.00	0.00	0.00	0.00	229.8	198.9	146.6	138.9	129.1	117.2	104.0	90.52
IS	0.00	0.00	0.00	0.00	0.51	0.59	1.07	1.13	1.22	1.34	1.52	1.75

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	9.37	9.41	9.46	9.53	9.61	9.72	9.80	9.86	9.94	10.04	10.17	10.31
mS	10.41	11.06	11.98	13.24	14.87	16.87	18.48	19.67	21.23	23.12	25.21	27.34
RE	7.18	6.76	6.23	5.64	5.02	4.43	4.04	3.80	3.52	3.23	2.96	2.73
t	18.55	18.57	18.60	18.64	18.70	18.80	22.35	22.45	22.61	22.86	23.26	23.93
RS	72.02	67.76	62.52	56.55	50.32	44.30	36.26	34.02	31.46	28.80	26.28	24.06
IS	2.12	2.26	2.45	2.71	3.05	3.46	3.57	3.80	4.10	4.46	4.84	5.20

427	$C_4H_8N_2O_3$			Gly-Gly				-31.5		8.400	132.1	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.84	7.87	7.91	7.97	8.04	8.13	8.33	8.37	8.44	8.52	8.62	8.74
mS	6.70	7.08	7.62	8.39	9.42	10.74	13.99	14.73	15.75	17.07	18.66	20.42
RE	11.15	10.55	9.80	8.90	7.93	6.95	5.34	5.07	4.74	4.38	4.00	3.66
t	25.85	25.86	25.87	25.88	25.90	25.92	18.70	18.70	18.70	18.71	18.71	18.73
RS	94.01	89.00	82.63	75.10	66.90	58.66	54.88	52.12	48.75	44.98	41.14	37.58
IS	1.37	1.44	1.56	1.72	1.93	2.21	3.31	3.49	3.74	4.07	4.46	4.90

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.76	8.85	8.95	9.08	9.24	9.41	9.33	9.48	9.65	9.83	10.03	10.23
mS	20.73	21.74	22.94	24.21	25.39	26.36	26.05	26.77	27.37	27.84	28.17	28.41
RE	3.60	3.44	3.26	3.09	2.94	2.83	2.87	2.79	2.73	2.68	2.65	2.63
t	19.55	19.57	19.59	19.62	19.68	19.78	23.82	23.93	24.13	24.44	24.98	25.90
RS	36.16	34.46	32.65	30.93	29.47	28.34	25.71	25.00	24.40	23.92	23.53	23.16
IS	4.88	5.13	5.42	5.73	6.01	6.23	5.68	5.83	5.94	6.01	6.02	5.96

428	$C_6H_{11}N_3O_4$			Gly-Gly-Gly				-26.1		8.102	189.2	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.70	7.74	7.79	7.86	7.94	8.04	8.21	8.26	8.34	8.44	8.56	8.71
mS	7.26	7.70	8.32	9.17	10.27	11.62	13.83	14.56	15.52	16.68	17.96	19.23
RE	10.29	9.70	8.98	8.15	7.27	6.43	5.40	5.13	4.81	4.48	4.16	3.88
t	29.37	29.38	29.40	29.43	29.46	29.50	20.69	20.69	20.70	20.71	20.73	20.76
RS	86.77	81.84	75.73	68.72	61.35	54.21	55.51	52.73	49.47	46.02	42.74	39.91
IS	1.59	1.69	1.83	2.02	2.27	2.57	3.63	3.83	4.09	4.41	4.76	5.11

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.68	8.78	8.92	9.07	9.25	9.43	9.33	9.50	9.69	9.88	10.09	10.30
mS	19.02	19.82	20.67	21.44	22.07	22.53	22.40	22.77	23.05	23.25	23.39	23.51
RE	3.93	3.77	3.61	3.48	3.39	3.31	3.34	3.28	3.24	3.21	3.19	3.18
t	21.75	21.78	21.82	21.87	21.97	22.12	27.02	27.21	27.53	28.05	28.96	30.60
RS	39.39	37.79	36.25	34.92	33.90	33.15	29.91	29.39	28.98	28.64	28.33	27.98
IS	4.93	5.14	5.37	5.57	5.73	5.83	5.26	5.33	5.36	5.35	5.28	5.14

429	$C_8H_{14}N_4O_5$			Gly-Gly-Gly-Gly				-23.3		8.142	246.2	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.73	7.77	7.82	7.89	7.97	8.07	8.23	8.29	8.37	8.47	8.59	8.74
mS	6.30	6.70	7.26	8.03	9.03	10.25	12.08	12.75	13.62	14.67	15.83	16.97
RE	11.86	11.15	10.28	9.30	8.27	7.29	6.18	5.86	5.48	5.09	4.72	4.40
t	31.84	31.86	31.89	31.92	31.97	32.03	22.12	22.13	22.14	22.16	22.19	22.23
RS	100.1	94.08	86.73	78.42	69.78	61.50	63.55	60.22	56.37	52.32	48.50	45.22
IS	1.43	1.52	1.65	1.83	2.06	2.35	3.34	3.53	3.78	4.08	4.42	4.75

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.71	8.81	8.95	9.10	9.28	9.47	9.37	9.54	9.73	9.93	10.13	10.35
mS	16.77	17.50	18.26	18.96	19.53	19.96	19.86	20.19	20.45	20.63	20.77	20.89
RE	4.46	4.27	4.09	3.94	3.82	3.74	3.76	3.70	3.65	3.62	3.60	3.58
t	23.35	23.39	23.44	23.52	23.64	23.84	29.36	29.62	30.05	30.78	32.07	34.52
RS	44.70	42.82	41.01	39.48	38.30	37.43	33.73	33.14	32.66	32.27	31.91	31.49
IS	4.56	4.77	4.98	5.17	5.32	5.41	4.84	4.90	4.92	4.89	4.80	4.60

430 $C_{10}H_{17}N_5O_6$ Gly-Gly-Gly-Gly-Gly -21.2 8.167 303.3

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.74	7.78	7.84	7.91	8.00	8.10	8.25	8.31	8.39	8.49	8.62	8.76
mS	5.63	6.01	6.54	7.25	8.17	9.29	10.85	11.47	12.27	13.24	14.30	15.34
RE	13.26	12.43	11.42	10.30	9.14	8.04	6.89	6.51	6.09	5.64	5.22	4.87
t	34.13	34.16	34.20	34.25	34.31	34.38	23.46	23.47	23.49	23.52	23.56	23.61
RS	111.9	104.9	96.36	86.87	77.11	67.84	70.78	66.96	62.56	57.98	53.69	50.04
IS	1.31	1.40	1.53	1.70	1.92	2.19	3.12	3.31	3.55	3.84	4.16	4.47

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.73	8.84	8.97	9.13	9.31	9.49	9.40	9.57	9.77	9.97	10.18	10.40
mS	15.13	15.81	16.51	17.15	17.66	18.05	17.98	18.28	18.51	18.68	18.82	18.94
RE	4.94	4.72	4.52	4.36	4.23	4.14	4.15	4.08	4.03	4.00	3.97	3.94
t	24.85	24.89	24.96	25.06	25.22	25.47	31.57	31.91	32.48	33.46	35.22	38.82
RS	49.53	47.39	45.36	43.66	42.35	41.39	37.26	36.59	36.07	35.64	35.22	34.73
IS	4.28	4.48	4.68	4.85	4.99	5.07	4.51	4.56	4.56	4.52	4.40	4.15

431 $C_{12}H_{20}N_6O_7$ Gly-Gly-Gly-Gly-Gly-Gly -19.3 8.107 360.3

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.72	7.76	7.82	7.90	7.99	8.10	8.23	8.29	8.38	8.49	8.62	8.77
mS	5.42	5.80	6.32	7.02	7.91	8.97	10.21	10.80	11.55	12.43	13.37	14.26
RE	13.78	12.89	11.82	10.64	9.44	8.33	7.32	6.92	6.47	6.01	5.59	5.24
t	36.68	36.72	36.77	36.83	36.91	37.00	24.94	24.96	24.99	25.03	25.07	25.14
RS	116.2	108.7	99.67	89.73	79.67	70.25	75.21	71.10	66.47	61.74	57.43	53.84
IS	1.30	1.39	1.52	1.69	1.91	2.17	3.06	3.24	3.47	3.75	4.04	4.32

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.72	8.84	8.98	9.15	9.33	9.52	9.43	9.61	9.80	10.01	10.22	10.46
mS	14.01	14.61	15.21	15.73	16.14	16.44	16.42	16.66	16.83	16.97	17.08	17.21
RE	5.33	5.11	4.91	4.75	4.63	4.54	4.55	4.48	4.44	4.40	4.37	4.34
t	26.50	26.56	26.64	26.77	26.97	27.29	34.03	34.48	35.23	36.55	39.05	44.68
RS	53.47	51.27	49.24	47.59	46.35	45.45	40.80	40.18	39.68	39.24	38.79	38.21
IS	4.11	4.29	4.47	4.61	4.72	4.77	4.23	4.25	4.23	4.16	4.00	3.68

432 $C_{10}H_{19}N_3O_4$ Gly-Gly-Ile -21.9 8.096 245.3

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.71	7.75	7.80	7.88	7.96	8.07	8.22	8.28	8.36	8.46	8.59	8.74
mS	6.17	6.57	7.14	7.90	8.88	10.06	11.64	12.29	13.13	14.12	15.18	16.21
RE	12.11	11.37	10.46	9.45	8.41	7.43	6.41	6.08	5.69	5.29	4.92	4.61
t	33.33	33.36	33.39	33.44	33.49	33.56	22.98	23.00	23.01	23.04	23.07	23.11
RS	102.2	95.89	88.27	79.74	70.97	62.65	65.94	62.47	58.50	54.39	50.57	47.35
IS	1.43	1.52	1.66	1.84	2.07	2.35	3.31	3.50	3.75	4.04	4.36	4.66

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.70	8.81	8.95	9.11	9.29	9.48	9.38	9.56	9.75	9.95	10.16	10.39
mS	15.97	16.64	17.33	17.94	18.42	18.78	18.72	19.00	19.21	19.37	19.49	19.60
RE	4.68	4.49	4.31	4.16	4.05	3.98	3.99	3.93	3.89	3.86	3.83	3.81
t	24.31	24.35	24.41	24.50	24.65	24.88	30.77	31.08	31.60	32.48	34.06	37.19
RS	46.93	45.02	43.23	41.73	40.60	39.78	35.79	35.22	34.77	34.38	34.01	33.56
IS	4.46	4.66	4.85	5.02	5.14	5.21	4.65	4.70	4.70	4.65	4.54	4.31

433 $C_{10}H_{19}N_3O_4$ Gly-Gly-Leu -21.9 8.116 245.3

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.72	7.76	7.81	7.88	7.97	8.07	8.22	8.28	8.37	8.47	8.60	8.74
mS	6.07	6.46	7.02	7.78	8.74	9.91	11.52	12.16	13.00	13.99	15.06	16.10
RE	12.32	11.56	10.64	9.61	8.55	7.54	6.48	6.14	5.75	5.34	4.96	4.64
t	33.33	33.35	33.39	33.43	33.49	33.55	22.98	23.00	23.01	23.04	23.07	23.11
RS	103.9	97.49	89.73	81.03	72.08	63.57	66.65	63.12	59.08	54.88	50.97	47.65
IS	1.40	1.50	1.63	1.81	2.04	2.32	3.27	3.46	3.71	4.00	4.32	4.63

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.71	8.82	8.95	9.12	9.29	9.48	9.38	9.56	9.75	9.95	10.16	10.39
mS	15.88	16.56	17.26	17.88	18.38	18.75	18.68	18.98	19.19	19.36	19.48	19.60
RE	4.71	4.51	4.33	4.18	4.06	3.98	4.00	3.94	3.89	3.86	3.83	3.81
t	24.31	24.35	24.41	24.51	24.65	24.88	30.78	31.09	31.60	32.48	34.06	37.19
RS	47.21	45.25	43.41	41.87	40.70	39.84	35.86	35.26	34.79	34.40	34.02	33.56
IS	4.44	4.63	4.83	5.00	5.13	5.20	4.64	4.69	4.69	4.65	4.54	4.31

434 $C_{13}H_{19}N_3O_4$ Gly-Gly-Phe -21.9 8.041 281.3

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.68	7.72	7.78	7.85	7.94	8.05	8.19	8.26	8.34	8.45	8.58	8.73
mS	6.45	6.87	7.46	8.25	9.26	10.46	11.98	12.64	13.48	14.46	15.50	16.48
RE	11.57	10.87	10.01	9.05	8.07	7.14	6.23	5.91	5.54	5.17	4.82	4.53
t	33.34	33.37	33.40	33.45	33.51	33.57	22.98	23.00	23.01	23.04	23.07	23.11
RS	97.62	91.65	84.42	76.35	68.07	60.24	64.07	60.75	56.97	53.10	49.53	46.57
IS	1.49	1.59	1.73	1.92	2.16	2.45	3.41	3.60	3.85	4.15	4.45	4.75

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.68	8.80	8.94	9.11	9.29	9.48	9.38	9.56	9.75	9.95	10.16	10.39
mS	16.21	16.87	17.52	18.09	18.53	18.85	18.80	19.06	19.25	19.39	19.50	19.61
RE	4.61	4.43	4.26	4.13	4.03	3.96	3.97	3.92	3.88	3.85	3.83	3.81
t	24.31	24.35	24.41	24.50	24.64	24.88	30.76	31.07	31.59	32.47	34.05	37.17
RS	46.22	44.42	42.75	41.39	40.36	39.63	35.63	35.10	34.69	34.33	33.98	33.54
IS	4.54	4.72	4.91	5.06	5.17	5.23	4.68	4.71	4.71	4.66	4.55	4.32

435 $C_9H_{17}N_3O_4$ Gly-Gly-Val -22.6 8.125 231.3

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.72	7.76	7.81	7.88	7.97	8.07	8.23	8.28	8.36	8.47	8.59	8.74
mS	6.20	6.60	7.17	7.93	8.92	10.11	11.83	12.49	13.34	14.36	15.47	16.56
RE	12.04	11.31	10.42	9.42	8.38	7.39	6.31	5.98	5.60	5.20	4.83	4.51
t	32.56	32.58	32.61	32.65	32.70	32.76	22.54	22.55	22.56	22.59	22.62	22.66
RS	101.6	95.41	87.89	79.43	70.67	62.31	64.90	61.49	57.56	53.46	49.61	46.34
IS	1.42	1.51	1.65	1.83	2.06	2.34	3.31	3.50	3.75	4.05	4.38	4.70

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.70	8.81	8.95	9.11	9.29	9.47	9.38	9.55	9.74	9.94	10.15	10.37
mS	16.34	17.05	17.78	18.44	18.97	19.36	19.28	19.59	19.83	20.00	20.13	20.24
RE	4.57	4.38	4.20	4.05	3.94	3.86	3.87	3.81	3.77	3.74	3.71	3.69
t	23.82	23.85	23.91	23.99	24.13	24.34	30.04	30.33	30.80	31.60	33.02	35.78
RS	45.86	43.95	42.13	40.61	39.44	38.59	34.75	34.16	33.69	33.30	32.93	32.49
IS	4.51	4.71	4.91	5.09	5.23	5.31	4.75	4.80	4.81	4.77	4.67	4.46

436 $C_{10}H_{15}N_5O_4$ Gly-His-Gly -22.5 8.279 269.3

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.79	7.83	7.88	7.95	8.03	8.13	8.29	8.35	8.42	8.52	8.63	8.77
mS	5.41	5.76	6.27	6.95	7.85	8.95	10.79	11.41	12.23	13.25	14.41	15.59
RE	13.81	12.96	11.92	10.74	9.52	8.34	6.92	6.55	6.11	5.64	5.18	4.79
t	32.64	32.66	32.69	32.73	32.78	32.84	22.60	22.61	22.63	22.65	22.69	22.73
RS	116.5	109.3	100.5	90.63	80.31	70.37	71.16	67.29	62.75	57.93	53.28	49.21
IS	1.24	1.32	1.44	1.60	1.81	2.07	3.02	3.20	3.44	3.73	4.07	4.42

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.76	8.85	8.98	9.13	9.30	9.48	9.40	9.56	9.75	9.94	10.15	10.37
mS	15.49	16.23	17.04	17.82	18.48	18.99	18.87	19.26	19.57	19.80	19.97	20.11
RE	4.82	4.60	4.38	4.19	4.04	3.93	3.96	3.88	3.82	3.77	3.74	3.71
t	23.90	23.93	23.99	24.08	24.22	24.44	30.18	30.46	30.94	31.75	33.20	36.01
RS	48.39	46.16	43.95	42.01	40.48	39.35	35.50	34.73	34.13	33.64	33.19	32.71
IS	4.27	4.48	4.71	4.92	5.09	5.21	4.64	4.72	4.75	4.73	4.63	4.43

437 $C_8H_{16}N_2O_3$ Gly-Ile -25.2 8.412 188.2

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.85	7.89	7.94	8.00	8.07	8.17	8.35	8.39	8.46	8.55	8.65	8.78
mS	5.35	5.68	6.16	6.83	7.71	8.82	11.12	11.75	12.61	13.71	15.00	16.41
RE	13.96	13.14	12.12	10.94	9.69	8.47	6.72	6.36	5.92	5.45	4.98	4.55
t	30.06	30.08	30.10	30.13	30.16	30.21	21.13	21.13	21.15	21.16	21.18	21.21
RS	117.8	110.8	102.2	92.30	81.76	71.42	69.05	65.34	60.88	56.00	51.16	46.76
IS	1.18	1.25	1.36	1.51	1.71	1.96	2.94	3.12	3.35	3.65	4.01	4.40

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.79	8.88	8.99	9.13	9.29	9.46	9.39	9.54	9.72	9.91	10.11	10.32
mS	16.51	17.36	18.33	19.33	20.23	20.96	20.77	21.32	21.77	22.11	22.36	22.55
RE	4.52	4.30	4.08	3.86	3.69	3.56	3.60	3.50	3.43	3.38	3.34	3.31
t	22.25	22.28	22.33	22.39	22.50	22.66	27.77	27.97	28.32	28.90	29.91	31.77
RS	45.39	43.17	40.86	38.73	36.98	35.64	32.25	31.39	30.68	30.12	29.64	29.17
IS	4.32	4.55	4.81	5.08	5.31	5.49	4.92	5.03	5.11	5.13	5.08	4.94

438 $C_8H_{16}N_2O_3$ Gly-Leu -25.1 8.432 188.2

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.86	7.90	7.94	8.01	8.08	8.17	8.36	8.40	8.47	8.55	8.66	8.79
mS	5.23	5.56	6.03	6.68	7.55	8.65	10.93	11.56	12.41	13.50	14.79	16.19
RE	14.27	13.43	12.38	11.18	9.90	8.64	6.83	6.46	6.02	5.53	5.05	4.61
t	30.15	30.16	30.18	30.21	30.25	30.29	21.18	21.19	21.20	21.21	21.23	21.27
RS	120.4	113.3	104.5	94.29	83.48	72.88	70.23	66.43	61.87	56.88	51.91	47.39
IS	1.15	1.23	1.33	1.48	1.68	1.92	2.90	3.07	3.30	3.60	3.96	4.35

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.80	8.88	8.99	9.13	9.29	9.47	9.39	9.55	9.72	9.91	10.11	10.32
mS	16.32	17.16	18.14	19.15	20.06	20.82	20.62	21.18	21.64	21.99	22.25	22.44
RE	4.58	4.35	4.12	3.90	3.72	3.59	3.62	3.53	3.45	3.40	3.36	3.33
t	22.31	22.34	22.38	22.45	22.56	22.72	27.85	28.06	28.41	29.00	30.02	31.91
RS	45.93	43.66	41.29	39.10	37.28	35.89	32.48	31.59	30.86	30.28	29.79	29.31
IS	4.27	4.50	4.77	5.03	5.27	5.46	4.89	5.01	5.08	5.10	5.06	4.92

439 $C_{11}H_{21}N_3O_4$ Gly-Leu-Ala -21.1 8.259 259.3

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.79	7.83	7.88	7.95	8.03	8.13	8.29	8.35	8.42	8.52	8.64	8.78
mS	5.18	5.53	6.02	6.69	7.56	8.62	10.24	10.84	11.63	12.60	13.67	14.77
RE	14.42	13.51	12.40	11.16	9.88	8.66	7.29	6.89	6.42	5.93	5.46	5.06
t	34.23	34.26	34.30	34.34	34.40	34.48	23.53	23.55	23.57	23.60	23.64	23.69
RS	121.6	114.0	104.6	94.17	83.37	73.07	74.95	70.81	66.00	60.95	56.13	51.97
IS	1.21	1.29	1.41	1.57	1.78	2.03	2.95	3.12	3.36	3.65	3.97	4.30

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.76	8.86	8.99	9.14	9.31	9.50	9.41	9.58	9.77	9.97	10.18	10.41
mS	14.62	15.32	16.07	16.77	17.36	17.80	17.72	18.07	18.33	18.53	18.69	18.83
RE	5.11	4.88	4.65	4.45	4.30	4.19	4.22	4.13	4.07	4.03	4.00	3.97
t	24.93	24.98	25.05	25.15	25.31	25.57	31.71	32.06	32.63	33.62	35.42	39.10
RS	51.25	48.90	46.61	44.64	43.10	41.96	37.81	37.04	36.43	35.93	35.46	34.94
IS	4.14	4.34	4.55	4.75	4.90	5.00	4.44	4.50	4.52	4.48	4.36	4.12

440 $C_{17}H_{25}N_3O_5$ Gly-Leu-Tyr* -21.0 8.405 351.4

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.86	7.90	7.95	8.01	8.10	8.19	8.35	8.41	8.48	8.57	8.68	8.81
mS	4.53	4.84	5.28	5.87	6.66	7.64	9.33	9.89	10.64	11.59	12.68	13.84
RE	16.50	15.44	14.16	12.72	11.22	9.78	8.01	7.55	7.02	6.45	5.89	5.40
t	34.33	34.35	34.39	34.44	34.50	34.57	23.61	23.62	23.65	23.68	23.72	23.77
RS	139.1	130.3	119.4	107.3	94.62	82.48	82.33	77.64	72.14	66.25	60.53	55.45
IS	1.05	1.13	1.23	1.37	1.56	1.80	2.68	2.84	3.07	3.35	3.68	4.03

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.81	8.90	9.02	9.17	9.33	9.51	9.44	9.60	9.78	9.98	10.19	10.41
mS	13.81	14.54	15.35	16.15	16.85	17.41	17.31	17.73	18.07	18.33	18.52	18.69
RE	5.41	5.14	4.87	4.63	4.43	4.29	4.32	4.21	4.13	4.08	4.03	4.00
t	25.03	25.08	25.15	25.26	25.42	25.69	31.87	32.22	32.81	33.82	35.65	39.43
RS	54.26	51.55	48.81	46.36	44.39	42.91	38.71	37.74	36.96	36.34	35.78	35.19
IS	3.90	4.11	4.34	4.57	4.76	4.89	4.34	4.42	4.45	4.43	4.32	4.08

441 $C_{11}H_{14}N_2O_3$ Gly-Phe -24.7 8.310 222.2

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.81	7.84	7.89	7.95	8.03	8.13	8.30	8.35	8.42	8.51	8.63	8.76
mS	5.75	6.11	6.63	7.34	8.27	9.44	11.62	12.27	13.15	14.25	15.52	16.85
RE	12.98	12.22	11.27	10.18	9.03	7.91	6.43	6.09	5.68	5.24	4.81	4.43
t	30.50	30.52	30.54	30.57	30.61	30.66	21.37	21.38	21.39	21.40	21.43	21.46
RS	109.5	103.0	95.04	85.86	76.18	66.75	66.09	62.57	58.39	53.89	49.48	45.55
IS	1.28	1.36	1.48	1.64	1.85	2.12	3.11	3.29	3.54	3.84	4.20	4.57

* The mobility was refined as a monoanion (a nonovalent anion).

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.76	8.85	8.97	9.11	9.28	9.46	9.38	9.54	9.72	9.91	10.11	10.33
mS	16.82	17.63	18.54	19.44	20.22	20.83	20.66	21.13	21.50	21.78	21.98	22.13
RE	4.44	4.24	4.03	3.84	3.69	3.59	3.61	3.53	3.47	3.43	3.40	3.37
t	22.52	22.55	22.59	22.66	22.77	22.95	28.15	28.37	28.74	29.35	30.43	32.41
RS	44.57	42.49	40.39	38.51	37.00	35.87	32.42	31.67	31.06	30.58	30.16	29.72
IS	4.45	4.67	4.92	5.16	5.36	5.50	4.93	5.03	5.08	5.08	5.02	4.86

442 $C_{20}H_{23}N_3O_4$ Gly-Phe-Phe -19.7 8.216 369.4

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.77	7.81	7.87	7.94	8.03	8.13	8.27	8.33	8.41	8.52	8.64	8.79
mS	5.04	5.39	5.88	6.54	7.39	8.42	9.81	10.39	11.15	12.05	13.05	14.03
RE	14.82	13.86	12.70	11.42	10.11	8.87	7.61	7.19	6.70	6.20	5.72	5.32
t	36.07	36.11	36.15	36.21	36.28	36.37	24.60	24.62	24.65	24.68	24.73	24.79
RS	125.0	116.9	107.2	96.34	85.28	74.83	78.26	73.89	68.88	63.69	58.83	54.69
IS	1.20	1.28	1.40	1.56	1.77	2.02	2.91	3.08	3.32	3.60	3.90	4.21

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.75	8.86	9.00	9.15	9.33	9.52	9.43	9.61	9.80	10.00	10.21	10.45
mS	13.84	14.49	15.16	15.77	16.27	16.65	16.60	16.89	17.11	17.28	17.42	17.56
RE	5.40	5.15	4.93	4.74	4.59	4.49	4.50	4.42	4.36	4.32	4.29	4.25
t	26.13	26.18	26.27	26.39	26.58	26.89	33.49	33.91	34.62	35.86	38.17	43.25
RS	54.13	51.71	49.40	47.46	45.97	44.88	40.36	39.61	39.02	38.53	38.05	37.46
IS	4.02	4.22	4.41	4.59	4.72	4.79	4.24	4.29	4.28	4.23	4.08	3.78

443 $C_7H_{12}N_2O_3$ Gly-Pro -27.8 8.746 172.2

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	8.01	8.04	8.09	8.14	8.21	8.29	8.50	8.54	8.59	8.66	8.75	8.86
mS	4.28	4.54	4.92	5.45	6.17	7.10	9.70	10.26	11.05	12.10	13.42	14.98
RE	17.43	16.44	15.19	13.71	12.11	10.51	7.70	7.28	6.76	6.17	5.57	4.99
t	28.09	28.10	28.11	28.13	28.16	28.19	20.03	20.03	20.04	20.05	20.07	20.09
RS	147.0	138.7	128.1	115.7	102.2	88.69	79.12	74.81	69.49	63.46	57.20	51.24
IS	0.91	0.96	1.04	1.16	1.31	1.52	2.43	2.57	2.77	3.04	3.39	3.79

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.91	8.98	9.07	9.19	9.32	9.48	9.44	9.57	9.72	9.90	10.09	10.29
mS	15.66	16.56	17.69	19.00	20.34	21.58	21.40	22.24	23.05	23.73	24.25	24.63
RE	4.77	4.51	4.22	3.93	3.67	3.46	3.49	3.36	3.24	3.15	3.08	3.03
t	21.04	21.06	21.10	21.15	21.23	21.37	26.00	26.16	26.43	26.88	27.64	28.99
RS	47.86	45.24	42.33	39.41	36.78	34.62	31.31	30.08	28.97	28.06	27.33	26.70
IS	3.88	4.11	4.40	4.74	5.07	5.38	4.87	5.05	5.21	5.32	5.36	5.30

444 $C_{10}H_{17}N_3O_4$ Gly-Pro-Ala -22.5 8.492 243.3

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.90	7.93	7.98	8.05	8.12	8.22	8.39	8.44	8.50	8.59	8.70	8.82
mS	4.46	4.76	5.18	5.76	6.53	7.51	9.43	10.00	10.77	11.75	12.91	14.18
RE	16.74	15.70	14.42	12.96	11.43	9.95	7.92	7.47	6.94	6.36	5.79	5.27
t	32.61	32.63	32.66	32.69	32.74	32.80	22.62	22.63	22.65	22.67	22.70	22.75
RS	141.2	132.4	121.6	109.3	96.43	83.90	81.40	76.80	71.32	65.36	59.45	54.11
IS	1.02	1.09	1.18	1.32	1.50	1.73	2.62	2.78	3.00	3.29	3.63	4.00

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.83	8.92	9.03	9.17	9.32	9.50	9.43	9.59	9.76	9.95	10.16	10.38
mS	14.29	15.06	15.96	16.89	17.74	18.44	18.30	18.81	19.25	19.58	19.83	20.02
RE	5.23	4.96	4.68	4.42	4.21	4.05	4.08	3.97	3.88	3.81	3.77	3.73
t	23.92	23.96	24.02	24.11	24.25	24.48	30.24	30.52	31.00	31.82	33.27	36.10
RS	52.46	49.75	46.93	44.33	42.17	40.51	36.62	35.56	34.70	34.01	33.43	32.85
IS	3.92	4.13	4.39	4.64	4.87	5.04	4.49	4.59	4.66	4.66	4.59	4.40

445 $C_5H_{10}N_2O_4$ Gly-Ser -28.1 8.350 162.1

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.82	7.85	7.90	7.96	8.03	8.12	8.31	8.36	8.43	8.51	8.62	8.75
mS	6.28	6.65	7.19	7.93	8.92	10.18	12.89	13.59	14.54	15.76	17.19	18.74
RE	11.89	11.23	10.39	9.42	8.37	7.34	5.80	5.50	5.14	4.74	4.34	3.99
t	27.89	27.90	27.91	27.93	27.96	27.99	19.86	19.87	19.87	19.88	19.89	19.91
RS	100.3	94.70	87.65	79.45	70.64	61.92	59.58	56.51	52.80	48.72	44.65	40.95
IS	1.34	1.42	1.53	1.69	1.91	2.18	3.24	3.42	3.67	3.99	4.37	4.78

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.76	8.84	8.96	9.09	9.25	9.43	9.35	9.50	9.68	9.87	10.07	10.27
mS	18.85	19.77	20.83	21.90	22.87	23.65	23.41	23.99	24.47	24.83	25.08	25.27
RE	3.96	3.78	3.59	3.41	3.27	3.16	3.19	3.11	3.05	3.01	2.98	2.95
t	20.84	20.86	20.89	20.94	21.02	21.15	25.70	25.85	26.11	26.54	27.27	28.57
RS	39.76	37.90	35.97	34.18	32.71	31.59	28.62	27.89	27.29	26.82	26.42	26.03
IS	4.70	4.93	5.21	5.48	5.72	5.91	5.34	5.46	5.54	5.58	5.55	5.45

446 $C_6H_{12}N_2O_4$ Gly-Thr -26.3 8.334 176.2

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.81	7.85	7.90	7.96	8.03	8.13	8.31	8.36	8.43	8.51	8.62	8.76
mS	5.98	6.34	6.87	7.59	8.55	9.75	12.19	12.86	13.77	14.93	16.27	17.71
RE	12.49	11.77	10.88	9.84	8.74	7.66	6.13	5.81	5.42	5.00	4.59	4.22
t	29.18	29.20	29.22	29.24	29.27	29.31	20.61	20.61	20.62	20.64	20.65	20.68
RS	105.4	99.30	91.75	83.01	73.72	64.59	63.01	59.70	55.75	51.43	47.17	43.33
IS	1.30	1.38	1.50	1.66	1.87	2.14	3.17	3.35	3.59	3.91	4.27	4.67

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.76	8.85	8.96	9.10	9.27	9.45	9.36	9.52	9.70	9.89	10.09	10.30
mS	17.75	18.62	19.60	20.58	21.45	22.15	21.95	22.47	22.89	23.21	23.44	23.61
RE	4.21	4.01	3.81	3.63	3.48	3.37	3.40	3.32	3.26	3.22	3.19	3.16
t	21.67	21.70	21.74	21.79	21.89	22.04	26.91	27.10	27.41	27.92	28.81	30.41
RS	42.22	40.25	38.22	36.38	34.87	33.73	30.53	29.78	29.17	28.69	28.28	27.86
IS	4.56	4.79	5.05	5.31	5.53	5.70	5.13	5.23	5.30	5.32	5.28	5.15

447 $C_{13}H_{15}N_3O_3$ Gly-Trp -23.6 8.359 261.3

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.83	7.87	7.92	7.98	8.06	8.15	8.33	8.38	8.45	8.54	8.65	8.78
mS	5.27	5.61	6.09	6.76	7.63	8.73	10.77	11.39	12.23	13.28	14.50	15.79
RE	14.17	13.31	12.26	11.05	9.78	8.55	6.93	6.56	6.11	5.63	5.15	4.73
t	31.51	31.53	31.55	31.59	31.63	31.68	21.96	21.97	21.98	22.00	22.03	22.07
RS	119.5	112.3	103.4	93.21	82.53	72.15	71.26	67.38	62.78	57.81	52.95	48.60
IS	1.19	1.26	1.38	1.53	1.73	1.99	2.94	3.12	3.35	3.65	4.00	4.37

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.78	8.87	8.99	9.13	9.30	9.48	9.40	9.56	9.74	9.93	10.13	10.35
mS	15.78	16.58	17.47	18.35	19.13	19.75	19.60	20.07	20.44	20.72	20.93	21.10
RE	4.73	4.51	4.28	4.07	3.90	3.78	3.81	3.72	3.65	3.60	3.57	3.54
t	23.18	23.21	23.27	23.34	23.47	23.66	29.13	29.38	29.79	30.50	31.73	34.08
RS	47.48	45.20	42.88	40.79	39.10	37.82	34.18	33.35	32.67	32.13	31.66	31.18
IS	4.25	4.47	4.72	4.96	5.17	5.31	4.75	4.84	4.89	4.89	4.82	4.64

448 $C_{12}H_{14}N_2O_5$ Gly-Tyr -19.7 -39.4 8.211 9.981 266.3

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.77	7.81	7.87	7.94	8.02	8.13	8.27	8.33	8.41	8.51	8.64	8.78
mS	5.12	5.47	5.98	6.66	7.54	8.62	10.17	10.80	11.64	12.67	13.87	15.16
RE	14.60	13.64	12.49	11.22	9.91	8.67	7.35	6.92	6.42	5.90	5.39	4.93
t	36.21	36.26	36.33	36.42	36.54	36.69	25.05	25.13	25.26	25.45	25.73	26.13
RS	123.1	115.1	105.4	94.61	83.58	73.11	75.52	71.10	65.99	60.59	55.36	50.64
IS	1.22	1.31	1.43	1.60	1.82	2.09	3.03	3.23	3.49	3.83	4.21	4.64

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.76	8.87	9.00	9.15	9.31	9.48	9.44	9.58	9.73	9.90	10.07	10.25
mS	15.03	15.93	17.02	18.24	19.62	21.14	20.84	22.16	23.64	25.22	26.81	28.29
RE	4.97	4.69	4.39	4.09	3.81	3.53	3.58	3.37	3.16	2.96	2.79	2.64
t	27.43	27.80	28.34	29.09	30.09	31.35	37.89	39.05	40.42	41.91	43.72	45.94
RS	49.88	47.02	44.02	41.03	38.13	35.34	32.15	30.20	28.25	26.41	24.72	23.25
IS	4.46	4.76	5.13	5.55	6.03	6.56	5.84	6.29	6.79	7.32	7.80	8.19

449 $C_7H_{14}N_2O_3$ Gly-Val -26.0 8.385 174.2

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.84	7.87	7.92	7.98	8.06	8.15	8.33	8.38	8.45	8.53	8.64	8.77
mS	5.65	6.00	6.49	7.18	8.10	9.26	11.67	12.32	13.21	14.34	15.68	17.12
RE	13.22	12.46	11.50	10.40	9.22	8.06	6.40	6.06	5.65	5.21	4.76	4.36
t	29.41	29.43	29.45	29.47	29.50	29.54	20.75	20.75	20.76	20.78	20.80	20.82
RS	111.5	105.1	97.01	87.70	77.78	68.03	65.80	62.30	58.11	53.52	48.96	44.82
IS	1.23	1.31	1.42	1.57	1.78	2.04	3.04	3.22	3.46	3.77	4.13	4.53

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.78	8.86	8.98	9.12	9.28	9.45	9.38	9.53	9.70	9.89	10.10	10.31
mS	17.21	18.08	19.07	20.08	20.99	21.73	21.53	22.08	22.53	22.87	23.12	23.30
RE	4.34	4.13	3.92	3.72	3.56	3.44	3.47	3.38	3.32	3.27	3.23	3.20
t	21.83	21.86	21.89	21.96	22.05	22.20	27.14	27.33	27.65	28.19	29.10	30.77
RS	43.54	41.45	39.27	37.28	35.63	34.38	31.12	30.31	29.64	29.11	28.67	28.23
IS	4.44	4.67	4.94	5.20	5.44	5.62	5.05	5.16	5.24	5.26	5.22	5.09

450	$C_6H_9N_3O_2$	Histidine	29.6 -28.8	6.040 9.342	155.2

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.84	7.87	7.92	7.98	8.06	8.15	8.79	8.82	8.86	8.92	9.00	9.09
mS	0.00	0.00	0.00	0.00	0.00	0.00	6.14	6.50	7.02	7.75	8.72	9.96
RE	0.00	0.00	0.00	0.00	0.00	0.00	12.17	11.49	10.64	9.64	8.57	7.50
t	0.00	0.00	0.00	0.00	0.00	0.00	20.01	20.00	19.99	19.98	19.98	19.99
RS	0.00	0.00	0.00	0.00	0.00	0.00	125.1	118.1	109.3	99.08	88.03	77.04
IS	0.00	0.00	0.00	0.00	0.00	0.00	1.47	1.56	1.69	1.87	2.11	2.42

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	9.18	9.23	9.29	9.38	9.48	9.61	9.64	9.73	9.84	9.98	10.14	10.32
mS	11.30	12.03	13.03	14.32	15.86	17.58	18.07	19.15	20.40	21.71	22.93	23.98
RE	6.61	6.21	5.73	5.22	4.71	4.25	4.13	3.90	3.66	3.44	3.26	3.11
t	20.92	20.94	20.97	21.03	21.12	21.25	25.82	25.99	26.25	26.68	27.41	28.69
RS	66.31	62.26	57.48	52.29	47.17	42.50	37.07	34.95	32.74	30.67	28.90	27.43
IS	2.69	2.87	3.11	3.43	3.80	4.21	3.97	4.20	4.47	4.72	4.93	5.03

451	$C_5H_9NO_3$	Hydroxyproline	-30.1	9.816	131.1

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.84	7.87	7.92	7.98	8.06	8.79	9.02	9.05	9.09	9.14	9.21	9.29
mS	0.00	0.00	0.00	0.00	0.00	2.57	4.13	4.37	4.72	5.22	5.91	6.81
RE	0.00	0.00	0.00	0.00	0.00	29.05	18.11	17.10	15.82	14.30	12.64	10.96
t	0.00	0.00	0.00	0.00	0.00	27.50	19.97	19.98	19.99	20.01	20.04	20.08
RS	0.00	0.00	0.00	0.00	0.00	245.0	186.1	175.8	162.6	147.0	129.9	112.7
IS	0.00	0.00	0.00	0.00	0.00	0.51	0.94	1.00	1.08	1.19	1.35	1.56

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	9.40	9.45	9.50	9.57	9.66	9.76	9.84	9.90	9.99	10.10	10.23	10.38
mS	8.25	8.80	9.58	10.62	11.97	13.60	14.87	15.88	17.19	18.75	20.46	22.18
RE	9.05	8.49	7.80	7.03	6.24	5.49	5.02	4.70	4.35	3.98	3.65	3.37
t	21.02	21.05	21.10	21.18	21.29	21.45	26.01	26.19	26.48	26.95	27.71	29.03
RS	90.82	85.12	78.21	70.48	62.52	54.92	45.06	42.13	38.86	35.52	32.39	29.66
IS	1.86	1.99	2.16	2.40	2.71	3.08	3.10	3.31	3.57	3.87	4.18	4.43

452	$C_6H_{13}NO_2$	Isoleucine	-26.7	9.765	131.2

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.84	7.87	7.92	7.98	8.06	8.79	9.00	9.03	9.07	9.13	9.20	9.28
mS	0.00	0.00	0.00	0.00	0.00	0.00	3.87	4.11	4.45	4.94	5.60	6.46
RE	0.00	0.00	0.00	0.00	0.00	0.00	19.29	18.18	16.77	15.13	13.35	11.57
t	0.00	0.00	0.00	0.00	0.00	0.00	21.29	21.30	21.32	21.34	21.38	21.43
RS	0.00	0.00	0.00	0.00	0.00	0.00	198.3	186.9	172.4	155.5	137.2	118.8
IS	0.00	0.00	0.00	0.00	0.00	0.00	0.94	0.99	1.08	1.20	1.36	1.57

No.	1.23	1.31	1.42	1.57	1.78	0.51	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	9.39	9.43	9.49	9.56	9.65	9.76	9.83	9.90	10.00	10.11	10.25	10.42
mS	7.70	8.22	8.96	9.95	11.21	12.71	13.75	14.70	15.90	17.30	18.79	20.26
RE	9.71	9.08	8.33	7.51	6.66	5.88	5.43	5.08	4.70	4.32	3.97	3.69
t	22.51	22.55	22.62	22.72	22.86	23.08	28.27	28.52	28.91	29.55	30.63	32.58
RS	97.39	91.10	83.56	75.22	66.74	58.76	48.72	45.52	42.01	38.49	35.26	32.47
IS	1.84	1.96	2.14	2.38	2.68	3.03	3.00	3.20	3.44	3.71	3.95	4.12

453	$C_6H_{13}NO_2$	Leucine	-26.4	9.728	131.2

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.84	7.87	7.92	7.98	8.06	8.76	8.98	9.01	9.06	9.11	9.18	9.27
mS	0.00	0.00	0.00	0.00	0.00	2.55	3.97	4.21	4.56	5.06	5.73	6.61
RE	0.00	0.00	0.00	0.00	0.00	29.30	18.83	17.74	16.37	14.76	13.03	11.29
t	0.00	0.00	0.00	0.00	0.00	29.96	21.36	21.37	21.39	21.41	21.45	21.50
RS	0.00	0.00	0.00	0.00	0.00	247.1	193.6	182.4	168.3	151.7	133.9	116.0
IS	0.00	0.00	0.00	0.00	0.00	0.53	0.97	1.03	1.11	1.24	1.40	1.62

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	9.37	9.41	9.47	9.55	9.64	9.75	9.82	9.89	9.98	10.10	10.25	10.41
mS	7.84	8.38	9.13	10.13	11.40	12.90	13.88	14.83	16.02	17.40	18.86	20.27
RE	9.53	8.92	8.18	7.37	6.55	5.79	5.38	5.04	4.66	4.29	3.96	3.68
t	22.58	22.63	22.69	22.79	22.94	23.16	28.39	28.64	29.03	29.68	30.77	32.76
RS	95.63	89.45	82.05	73.90	65.64	57.89	48.27	45.12	41.68	38.26	35.14	32.46
IS	1.89	2.02	2.20	2.44	2.75	3.11	3.05	3.25	3.49	3.75	4.00	4.15

454 $C_8H_{16}N_2O_4$ Leu-Gly -25.0 8.269 204.2

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.78	7.82	7.87	7.93	8.01	8.11	8.28	8.33	8.41	8.50	8.61	8.75
mS	6.03	6.41	6.95	7.68	8.65	9.85	12.05	12.72	13.62	14.73	16.01	17.34
RE	12.38	11.65	10.75	9.72	8.64	7.58	6.20	5.87	5.49	5.07	4.67	4.31
t	30.25	30.27	30.29	30.32	30.35	30.40	21.22	21.22	21.23	21.25	21.27	21.30
RS	104.4	98.28	90.71	82.02	72.86	63.94	63.71	60.35	56.39	52.11	47.95	44.27
IS	1.34	1.42	1.54	1.71	1.93	2.20	3.21	3.40	3.65	3.96	4.31	4.68

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.74	8.83	8.96	9.10	9.27	9.45	9.37	9.53	9.71	9.90	10.11	10.32
mS	17.27	18.08	18.99	19.86	20.61	21.19	21.03	21.48	21.83	22.09	22.28	22.43
RE	4.33	4.13	3.93	3.76	3.62	3.52	3.55	3.48	3.42	3.38	3.35	3.33
t	22.35	22.38	22.42	22.49	22.59	22.76	27.90	28.11	28.46	29.06	30.09	31.99
RS	43.40	41.43	39.45	37.70	36.29	35.25	31.85	31.15	30.59	30.14	29.75	29.33
IS	4.55	4.77	5.01	5.25	5.44	5.58	5.00	5.09	5.14	5.14	5.08	4.92

455 $C_{10}H_{19}N_3O_4$ Leu-Gly-Gly -21.5 7.992 245.3

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.66	7.70	7.76	7.83	7.93	8.03	8.17	8.24	8.33	8.44	8.57	8.73
mS	6.60	7.03	7.63	8.44	9.45	10.65	12.06	12.71	13.54	14.49	15.48	16.40
RE	11.32	10.62	9.79	8.86	7.91	7.01	6.19	5.88	5.52	5.15	4.82	4.55
t	33.82	33.85	33.88	33.93	33.99	34.06	23.25	23.27	23.28	23.31	23.34	23.39
RS	95.48	89.62	82.55	74.70	66.68	59.15	63.67	60.40	56.71	52.97	49.57	46.78
IS	1.54	1.64	1.78	1.98	2.22	2.51	3.46	3.66	3.91	4.19	4.49	4.77

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.67	8.79	8.94	9.11	9.29	9.48	9.38	9.56	9.75	9.96	10.17	10.40
mS	16.12	16.74	17.35	17.87	18.27	18.55	18.52	18.75	18.92	19.04	19.15	19.25
RE	4.63	4.46	4.31	4.18	4.09	4.03	4.03	3.98	3.95	3.92	3.90	3.88
t	24.60	24.65	24.71	24.81	24.96	25.20	31.20	31.53	32.07	33.00	34.68	38.06
RS	46.49	44.75	43.17	41.90	40.95	40.27	36.18	35.69	35.30	34.96	34.61	34.17
IS	4.55	4.73	4.90	5.04	5.14	5.19	4.63	4.66	4.65	4.60	4.47	4.23

456 $C_{17}H_{25}N_3O_4$ Leu-Gly-Phe -19.3 7.938 335.4

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.64	7.69	7.75	7.83	7.92	8.04	8.16	8.23	8.32	8.44	8.59	8.75
mS	6.22	6.64	7.23	8.00	8.95	10.06	11.11	11.72	12.47	13.32	14.16	14.92
RE	12.02	11.25	10.34	9.34	8.34	7.42	6.72	6.37	5.99	5.61	5.27	5.01
t	36.74	36.78	36.83	36.89	36.97	37.06	24.95	24.97	24.99	25.03	25.08	25.13
RS	101.4	94.89	87.19	78.79	70.37	62.61	69.09	65.50	61.55	57.64	54.19	51.43
IS	1.49	1.60	1.74	1.93	2.17	2.45	3.34	3.53	3.77	4.03	4.30	4.53

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.68	8.80	8.96	9.13	9.32	9.51	9.41	9.60	9.80	10.00	10.22	10.46
mS	14.64	15.18	15.67	16.08	16.39	16.61	16.62	16.80	16.93	17.03	17.12	17.24
RE	5.10	4.92	4.77	4.64	4.56	4.50	4.49	4.45	4.41	4.39	4.36	4.33
t	26.49	26.55	26.63	26.76	26.96	27.28	34.00	34.45	35.20	36.52	39.01	44.63
RS	51.19	49.37	47.79	46.54	45.64	44.98	40.31	39.84	39.46	39.11	38.71	38.16
IS	4.31	4.47	4.61	4.73	4.80	4.82	4.28	4.29	4.26	4.18	4.02	3.69

457 $C_{12}H_{24}N_2O_3$ Leu-Leu -21.6 8.397 244.3

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.85	7.89	7.94	8.01	8.09	8.18	8.35	8.40	8.47	8.56	8.67	8.81
mS	4.68	5.00	5.45	6.06	6.86	7.87	9.64	10.21	10.98	11.95	13.08	14.27
RE	15.95	14.94	13.71	12.33	10.88	9.49	7.75	7.31	6.80	6.25	5.71	5.24
t	33.62	33.64	33.67	33.72	33.77	33.84	23.19	23.20	23.22	23.25	23.29	23.34
RS	134.5	126.0	115.7	104.0	91.81	80.07	79.67	75.18	69.89	64.22	58.70	53.79
IS	1.08	1.16	1.26	1.41	1.60	1.84	2.73	2.90	3.13	3.42	3.75	4.10

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.80	8.89	9.01	9.16	9.32	9.50	9.43	9.59	9.77	9.97	10.17	10.40
mS	14.25	14.99	15.82	16.64	17.37	17.94	17.83	18.26	18.61	18.87	19.07	19.24
RE	5.24	4.98	4.72	4.49	4.30	4.16	4.19	4.09	4.01	3.96	3.92	3.88
t	24.56	24.60	24.67	24.77	24.92	25.17	31.17	31.50	32.03	32.96	34.62	37.96
RS	52.60	49.99	47.35	44.99	43.07	41.64	37.58	36.64	35.89	35.28	34.75	34.18
IS	3.98	4.19	4.43	4.66	4.85	4.99	4.43	4.52	4.56	4.54	4.44	4.22

458 $C_{18}H_{35}N_3O_4$ Leu-Leu-Leu -17.6 7.730 357.5

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.55	7.60	7.67	7.76	7.87	8.00	8.09	8.17	8.28	8.42	8.57	8.75
mS	6.66	7.12	7.75	8.54	9.48	10.51	11.10	11.67	12.33	13.01	13.64	14.15
RE	11.21	10.49	9.64	8.75	7.88	7.11	6.73	6.40	6.06	5.74	5.48	5.28
t	39.60	39.65	39.72	39.80	39.90	40.00	26.59	26.61	26.65	26.69	26.75	26.82
RS	94.58	88.46	81.35	73.80	66.48	59.94	69.19	65.82	62.29	59.00	56.28	54.22
IS	1.65	1.76	1.92	2.12	2.36	2.62	3.47	3.66	3.87	4.10	4.30	4.47

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.65	8.79	8.96	9.15	9.34	9.54	9.44	9.63	9.84	10.05	10.27	10.54
mS	13.90	14.29	14.63	14.88	15.06	15.19	15.24	15.35	15.43	15.50	15.58	15.72
RE	5.37	5.23	5.11	5.02	4.96	4.92	4.90	4.87	4.84	4.82	4.79	4.75
t	28.30	28.37	28.47	28.63	28.88	29.29	36.70	37.29	38.30	40.12	43.77	53.65
RS	53.90	52.42	51.21	50.32	49.67	49.20	43.95	43.60	43.29	42.96	42.54	41.85
IS	4.24	4.36	4.46	4.52	4.55	4.54	4.02	4.00	3.95	3.84	3.63	3.18

459 $C_{15}H_{22}N_2O_3$ Leu-Phe -21.8 8.413 278.4

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.86	7.90	7.95	8.01	8.09	8.19	8.35	8.41	8.48	8.57	8.68	8.81
mS	4.66	4.97	5.41	6.02	6.82	7.82	9.63	10.20	10.97	11.95	13.08	14.29
RE	16.04	15.03	13.80	12.40	10.95	9.55	7.76	7.32	6.81	6.25	5.71	5.23
t	33.38	33.41	33.44	33.48	33.54	33.60	23.06	23.07	23.09	23.12	23.15	23.20
RS	135.3	126.8	116.4	104.6	92.37	80.53	79.76	75.26	69.96	64.25	58.68	53.71
IS	1.07	1.15	1.25	1.39	1.58	1.82	2.72	2.89	3.11	3.40	3.73	4.09

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.81	8.90	9.02	9.16	9.32	9.50	9.43	9.59	9.77	9.96	10.17	10.39
mS	14.29	15.04	15.88	16.73	17.47	18.07	17.95	18.40	18.76	19.04	19.25	19.42
RE	5.23	4.97	4.70	4.47	4.27	4.13	4.16	4.06	3.98	3.92	3.88	3.85
t	24.41	24.46	24.52	24.62	24.77	25.01	30.96	31.27	31.79	32.69	34.30	37.52
RS	52.45	49.82	47.16	44.76	42.81	41.34	37.32	36.37	35.59	34.97	34.43	33.87
IS	3.98	4.19	4.43	4.66	4.86	5.01	4.45	4.54	4.58	4.57	4.48	4.26

460 $C_{15}H_{22}N_2O_4$ Leu-Tyr -18.2 7.828 294.3
-36.4 10.065

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.60	7.64	7.71	7.79	7.90	8.01	8.12	8.20	8.30	8.43	8.58	8.74
mS	6.44	6.88	7.50	8.29	9.26	10.36	11.22	11.84	12.61	13.46	14.34	15.20
RE	11.61	10.85	9.96	9.01	8.07	7.21	6.66	6.31	5.93	5.55	5.21	4.92
t	38.59	38.65	38.72	38.82	38.95	39.10	26.24	26.31	26.43	26.61	26.87	27.25
RS	97.90	91.53	84.05	76.00	68.05	60.81	68.44	64.83	60.91	57.04	53.54	50.50
IS	1.58	1.69	1.84	2.05	2.29	2.58	3.48	3.68	3.93	4.22	4.52	4.82

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.67	8.81	8.97	9.14	9.32	9.50	9.44	9.60	9.76	9.93	10.10	10.29
mS	14.87	15.54	16.30	17.15	18.14	19.31	19.03	20.15	21.42	22.82	24.26	25.66
RE	5.02	4.81	4.58	4.35	4.12	3.87	3.92	3.71	3.49	3.27	3.08	2.91
t	28.55	28.92	29.47	30.25	31.29	32.63	39.61	41.00	42.56	44.36	46.43	49.17
RS	50.41	48.20	45.95	43.65	41.24	38.69	35.20	33.22	31.18	29.18	27.32	25.63
IS	4.55	4.79	5.06	5.37	5.74	6.17	5.45	5.83	6.28	6.74	7.19	7.53

461 $C_{11}H_{22}N_2O_3$ Leu-Val -22.3 8.364 230.3

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.84	7.87	7.92	7.99	8.07	8.17	8.33	8.38	8.45	8.55	8.66	8.79
mS	4.97	5.30	5.77	6.41	7.25	8.30	10.15	10.75	11.55	12.55	13.71	14.92
RE	15.02	14.09	12.95	11.65	10.30	9.00	7.36	6.95	6.47	5.95	5.45	5.01
t	32.84	32.86	32.89	32.93	32.98	33.04	22.73	22.74	22.76	22.79	22.82	22.86
RS	126.7	118.8	109.2	98.30	86.91	75.91	75.61	71.42	66.48	61.17	56.01	51.43
IS	1.14	1.22	1.32	1.47	1.67	1.92	2.84	3.02	3.25	3.54	3.88	4.24

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.79	8.88	9.00	9.15	9.31	9.49	9.41	9.57	9.76	9.95	10.16	10.38
mS	14.89	15.65	16.49	17.32	18.05	18.62	18.50	18.93	19.28	19.54	19.73	19.90
RE	5.02	4.77	4.53	4.31	4.14	4.01	4.04	3.95	3.87	3.82	3.78	3.75
t	24.05	24.08	24.14	24.24	24.38	24.60	30.40	30.70	31.19	32.02	33.51	36.44
RS	50.33	47.89	45.43	43.22	41.45	40.12	36.22	35.35	34.64	34.08	33.58	33.06
IS	4.11	4.32	4.56	4.79	4.98	5.12	4.56	4.64	4.68	4.67	4.58	4.37

462 $C_6H_{14}N_2O_2$ Lysine

463 $C_5H_{11}NO_2S$ Methionine -30.4 9.376 149.2

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.84	8.35	8.39	8.44	8.50	8.57	8.80	8.83	8.87	8.93	9.00	9.09
mS	0.00	2.61	2.82	3.12	3.53	4.10	6.27	6.63	7.16	7.90	8.89	10.16
RE	0.00	28.67	26.53	23.97	21.13	18.23	11.92	11.27	10.43	9.46	8.41	7.35
t	0.00	26.67	26.68	26.69	26.71	26.73	19.33	19.34	19.34	19.35	19.37	19.40
RS	126.7	241.9	223.8	202.2	178.3	153.8	122.6	115.8	107.2	97.22	86.38	75.57
IS	1.14	0.53	0.57	0.63	0.72	0.83	1.46	1.55	1.68	1.85	2.09	2.39

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	9.19	9.24	9.30	9.38	9.48	9.61	9.65	9.73	9.84	9.97	10.13	10.30
mS	11.62	12.37	13.39	14.72	16.32	18.14	18.74	19.86	21.18	22.60	23.95	25.11
RE	6.43	6.04	5.58	5.08	4.58	4.12	3.99	3.76	3.53	3.31	3.12	2.97
t	20.28	20.30	20.34	20.39	20.47	20.60	24.92	25.06	25.29	25.66	26.29	27.38
RS	64.48	60.58	55.94	50.88	45.83	41.19	35.76	33.70	31.53	29.47	27.67	26.19
IS	2.70	2.87	3.11	3.43	3.81	4.24	4.03	4.27	4.54	4.82	5.06	5.20

464 $C_5H_{12}N_2O_2$ Ornithine 28.4 8.712 132.2 -28.4 10.755

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.84	8.35	8.39	8.44	8.50	8.57	8.80	8.83	8.87	8.93	9.00	9.09
mS	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
RE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
t	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
RS	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
IS	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	9.19	9.24	9.30	9.38	9.48	10.32	9.65	9.73	10.56	10.64	10.74	10.90
mS	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	10.50	11.69	13.36	15.90
RE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	7.12	6.39	5.59	4.70
t	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	56.00	60.38	70.55	112.2
RS	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	63.62	56.95	49.60	41.37
IS	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.43	1.53	1.62	1.60

465 $C_9H_{11}NO_2$ Phenylalanine -26.9 9.262 165.2

No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.84	8.30	8.34	8.39	8.46	8.53	8.75	8.78	8.83	8.89	8.97	9.06
mS	0.00	2.62	2.85	3.16	3.60	4.18	6.16	6.54	7.07	7.81	8.79	10.02
RE	0.00	28.47	26.25	23.62	20.76	17.88	12.12	11.43	10.56	9.56	8.50	7.45
t	0.00	28.89	28.90	28.92	28.95	28.98	20.59	20.60	20.61	20.63	20.65	20.69
RS	126.7	240.2	221.4	199.3	175.1	150.8	124.6	117.5	108.6	98.30	87.34	76.57
IS	1.14	0.56	0.60	0.67	0.76	0.89	1.53	1.63	1.77	1.96	2.21	2.52

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	9.14	9.20	9.27	9.36	9.47	9.60	9.62	9.71	9.83	9.98	10.15	10.33
mS	11.18	11.91	12.90	14.14	15.61	17.20	17.52	18.53	19.67	20.82	21.86	22.72
RE	6.68	6.27	5.79	5.28	4.79	4.34	4.26	4.03	3.80	3.59	3.42	3.29
t	21.69	21.72	21.77	21.84	21.94	22.10	27.00	27.19	27.50	28.02	28.90	30.48
RS	67.04	62.90	58.08	52.94	47.93	43.45	38.23	36.11	33.95	31.98	30.32	28.95
IS	2.76	2.94	3.19	3.51	3.87	4.27	3.96	4.18	4.42	4.64	4.80	4.84

466	$C_5H_9O_2N$			Proline				-29.0		10.640		115.1	
No.	32	33	34	35	36	37	38	39	40	41	42	43	
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40	
pHS	7.84	8.30	8.34	8.39	8.46	8.53	8.75	8.78	8.83	8.89	9.67	9.74	
mS	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	2.78	3.21	
RE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	26.92	23.28	
t	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	27.32	27.50	
RS	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	276.6	239.2	
IS	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.52	0.60	
No.	44	45	46	47	48	49	50	51	52	53	54	55	
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00	
pHS	9.89	9.92	9.96	10.02	10.09	10.18	10.33	10.37	10.43	10.51	10.62	10.75	
mS	4.33	4.60	4.99	5.55	6.31	7.31	9.30	9.93	10.83	12.06	13.67	15.74	
RE	17.26	16.25	14.97	13.47	11.84	10.22	8.03	7.52	6.89	6.19	5.46	4.74	
t	29.12	29.26	29.48	29.81	30.30	31.04	38.51	39.30	40.59	42.75	46.67	55.15	
RS	173.2	163.0	150.1	135.0	118.6	102.2	72.05	67.35	61.64	55.21	48.48	41.78	
IS	0.79	0.83	0.90	1.00	1.13	1.29	1.52	1.61	1.72	1.87	2.03	2.15	

467	$C_3H_7NO_3$			Serine				-34.3		9.329		105.1	
No.	32	33	34	35	36	37	38	39	40	41	42	43	
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40	
pHS	8.29	8.32	8.36	8.40	8.46	8.54	8.77	8.80	8.84	8.90	8.97	9.06	
mS	2.90	3.06	3.29	3.63	4.10	4.74	7.35	7.76	8.35	9.19	10.31	11.76	
RE	25.78	24.44	22.69	20.58	18.21	15.76	10.17	9.63	8.94	8.13	7.24	6.35	
t	24.64	24.65	24.65	24.66	24.67	24.69	18.14	18.15	18.15	18.16	18.17	18.18	
RS	217.5	206.1	191.4	173.6	153.6	133.0	104.5	98.96	91.90	83.54	74.44	65.29	
IS	0.56	0.59	0.64	0.70	0.80	0.92	1.61	1.71	1.84	2.03	2.28	2.61	
No.	44	45	46	47	48	49	50	51	52	53	54	55	
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00	
pHS	9.16	9.21	9.27	9.35	9.45	9.57	9.61	9.69	9.80	9.93	10.08	10.26	
mS	13.50	14.33	15.47	16.96	18.77	20.80	21.45	22.68	24.15	25.72	27.21	28.50	
RE	5.53	5.21	4.83	4.40	3.98	3.59	3.48	3.29	3.09	2.90	2.74	2.62	
t	18.96	18.97	18.99	19.03	19.09	19.18	22.96	23.06	23.23	23.50	23.94	24.70	
RS	55.52	52.28	48.40	44.14	39.86	35.91	31.23	29.50	27.65	25.89	24.35	23.08	
IS	2.96	3.14	3.40	3.73	4.14	4.60	4.41	4.67	4.96	5.27	5.54	5.73	

468	$C_9H_{17}N_3O_7$			Ser-Ser-Ser				-22.0		7.385		279.3	
No.	32	33	34	35	36	37	38	39	40	41	42	43	
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40	
pHS	7.38	7.44	7.51	7.60	7.72	7.86	7.94	8.04	8.16	8.31	8.48	8.66	
mS	10.39	11.01	11.83	12.84	13.99	15.19	15.69	16.33	17.02	17.68	18.23	18.65	
RE	7.19	6.79	6.32	5.82	5.34	4.92	4.76	4.57	4.39	4.23	4.10	4.01	
t	33.41	33.44	33.48	33.52	33.58	33.63	22.93	22.94	22.96	22.98	23.00	23.04	
RS	60.62	57.23	53.28	49.07	45.03	41.49	48.93	47.03	45.11	43.43	42.10	41.15	
IS	2.43	2.58	2.78	3.02	3.30	3.59	4.51	4.70	4.91	5.11	5.28	5.40	
No.	44	45	46	47	48	49	50	51	52	53	54	55	
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00	
pHS	8.54	8.70	8.88	9.07	9.26	9.46	9.34	9.53	9.73	9.94	10.15	10.38	
mS	18.40	18.74	19.00	19.19	19.32	19.41	19.47	19.55	19.60	19.65	19.70	19.77	
RE	4.06	3.99	3.93	3.89	3.87	3.85	3.84	3.82	3.81	3.80	3.79	3.78	
t	24.22	24.26	24.31	24.40	24.54	24.77	30.61	30.91	31.42	32.29	33.83	36.89	
RS	40.72	39.98	39.42	39.01	38.72	38.49	34.41	34.23	34.07	33.89	33.64	33.28	
IS	5.18	5.27	5.34	5.38	5.40	5.39	4.85	4.84	4.80	4.73	4.60	4.36	

469	$C_2H_7NO_3S$			Taurine				-37.9		9.182		125.1	
No.	32	33	34	35	36	37	38	39	40	41	42	43	
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40	
pHS	8.22	8.24	8.28	8.32	8.38	8.46	8.69	8.73	8.77	8.83	8.90	8.99	
mS	3.71	3.91	4.20	4.61	5.19	5.98	9.23	9.73	10.45	11.45	12.80	14.51	
RE	20.12	19.11	17.80	16.19	14.38	12.49	8.09	7.68	7.15	6.52	5.84	5.15	
t	23.12	23.13	23.13	23.14	23.14	23.16	17.24	17.24	17.24	17.24	17.25	17.26	
RS	169.7	161.2	150.1	136.6	121.3	105.4	83.20	78.94	73.50	67.04	59.98	52.88	
IS	0.69	0.73	0.78	0.86	0.97	1.12	1.93	2.04	2.19	2.41	2.70	3.07	
No.	44	45	46	47	48	49	50	51	52	53	54	55	
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00	
pHS	9.09	9.13	9.20	9.28	9.39	9.52	9.54	9.63	9.74	9.88	10.04	10.21	
mS	16.45	17.41	18.73	20.42	22.44	24.66	25.12	26.45	28.00	29.59	31.05	32.26	
RE	4.54	4.29	3.99	3.66	3.33	3.03	2.97	2.82	2.67	2.52	2.41	2.32	
t	17.94	17.95	17.97	18.00	18.04	18.10	21.48	21.56	21.68	21.89	22.22	22.79	
RS	45.56	43.02	39.99	36.66	33.33	30.30	26.67	25.30	23.86	22.50	21.34	20.39	
IS	3.44	3.64	3.93	4.29	4.73	5.20	4.98	5.24	5.55	5.86	6.12	6.31	

470	$C_4H_9NO_3$			Threonine					-31.6	9.229	119.1	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	8.25	8.27	8.31	8.36	8.42	8.50	8.72	8.76	8.80	8.86	8.94	9.03
mS	2.97	3.14	3.39	3.75	4.25	4.91	7.41	7.84	8.45	9.30	10.43	11.87
RE	25.12	23.76	22.01	19.91	17.59	15.21	10.08	9.53	8.84	8.03	7.16	6.29
t	25.92	25.92	25.93	25.94	25.96	25.98	18.86	18.86	18.87	18.88	18.89	18.91
RS	211.8	200.4	185.6	168.0	148.4	128.3	103.6	97.96	90.86	82.55	73.59	64.67
IS	0.60	0.63	0.68	0.75	0.85	0.99	1.71	1.81	1.95	2.15	2.42	2.76

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	9.12	9.17	9.23	9.32	9.43	9.56	9.58	9.67	9.79	9.93	10.09	10.27
mS	13.35	14.18	15.31	16.74	18.44	20.30	20.69	21.84	23.16	24.51	25.74	26.75
RE	5.59	5.27	4.88	4.46	4.05	3.68	3.61	3.42	3.22	3.05	2.90	2.79
t	19.75	19.77	19.80	19.84	19.91	20.01	24.12	24.25	24.45	24.77	25.32	26.27
RS	56.13	52.83	48.93	44.72	40.56	36.80	32.38	30.64	28.84	27.17	25.75	24.59
IS	3.06	3.26	3.52	3.86	4.26	4.69	4.42	4.66	4.93	5.20	5.41	5.53

471	$C_{11}H_{12}N_2O_2$			Tryptophan					-26.8	9.635	204.2	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	8.25	8.27	8.31	8.36	8.42	8.71	8.93	8.97	9.01	9.07	9.14	9.22
mS	0.00	0.00	0.00	0.00	0.00	2.84	4.38	4.65	5.04	5.58	6.32	7.28
RE	0.00	0.00	0.00	0.00	0.00	26.30	17.04	16.06	14.82	13.38	11.82	10.26
t	0.00	0.00	0.00	0.00	0.00	29.46	21.01	21.02	21.04	21.06	21.09	21.14
RS	0.00	0.00	0.00	0.00	0.00	221.9	175.2	165.1	152.3	137.5	121.4	105.5
IS	0.00	0.00	0.00	0.00	0.00	0.60	1.07	1.14	1.23	1.37	1.55	1.79

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	9.32	9.37	9.43	9.51	9.60	9.71	9.77	9.85	9.95	10.07	10.22	10.39
mS	8.53	9.11	9.92	10.99	12.32	13.89	14.75	15.73	16.95	18.32	19.73	21.05
RE	8.76	8.20	7.53	6.80	6.06	5.38	5.06	4.75	4.41	4.08	3.78	3.55
t	22.18	22.22	22.28	22.37	22.50	22.70	27.78	28.00	28.36	28.95	29.94	31.73
RS	87.86	82.23	75.51	68.15	60.72	53.80	45.42	42.53	39.40	36.34	33.58	31.24
IS	2.06	2.20	2.40	2.66	2.98	3.36	3.25	3.46	3.71	3.98	4.22	4.36

472	$C_9H_{11}NO_3$			Tyrosine					-20.7 -42.0	9.165 10.207	181.2	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	8.25	8.27	8.31	8.37	8.44	8.52	8.71	8.75	8.80	8.87	8.95	9.05
mS	0.00	0.00	2.56	2.88	3.30	3.87	5.51	5.90	6.44	7.20	8.20	9.48
RE	0.00	0.00	29.16	25.97	22.60	19.29	13.55	12.67	11.59	10.38	9.11	7.88
t	0.00	0.00	35.12	35.20	35.30	35.44	24.69	24.77	24.88	25.04	25.27	25.59
RS	0.00	0.00	246.0	219.1	190.7	162.7	139.2	130.2	119.1	106.6	93.61	81.00
IS	0.00	0.00	0.59	0.67	0.77	0.90	1.56	1.67	1.83	2.06	2.35	2.74

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	9.12	9.17	9.25	9.34	9.46	9.59	9.61	9.70	9.82	9.95	10.10	10.27
mS	10.47	11.30	12.43	13.89	15.68	17.76	18.20	19.69	21.52	23.58	25.74	27.86
RE	7.13	6.61	6.01	5.38	4.76	4.20	4.10	3.79	3.47	3.17	2.90	2.68
t	27.14	27.38	27.74	28.25	28.94	29.85	36.48	37.28	38.40	39.76	41.40	43.55
RS	71.57	66.30	60.26	53.90	47.70	42.06	36.82	33.98	31.03	28.24	25.75	23.61
IS	2.96	3.21	3.55	4.00	4.55	5.20	4.87	5.31	5.85	6.47	7.11	7.69

473	$C_5H_{11}NO_2$			Valine					-28.4	9.710	117.1	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	8.25	8.27	8.31	8.37	8.44	8.74	8.97	9.00	9.04	9.10	9.17	9.25
mS	0.00	0.00	0.00	0.00	0.00	2.75	4.32	4.58	4.95	5.48	6.20	7.15
RE	0.00	0.00	0.00	0.00	0.00	27.20	17.31	16.33	15.08	13.63	12.04	10.45
t	0.00	0.00	0.00	0.00	0.00	28.41	20.44	20.45	20.46	20.48	20.51	20.55
RS	0.00	0.00	0.00	0.00	0.00	229.4	177.9	167.8	155.0	140.0	123.8	107.4
IS	0.00	0.00	0.00	0.00	0.00	0.56	1.02	1.08	1.17	1.30	1.47	1.70

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	9.36	9.40	9.46	9.53	9.62	9.73	9.80	9.87	9.96	10.08	10.22	10.38
mS	8.50	9.07	9.87	10.94	12.29	13.91	14.95	15.96	17.23	18.70	20.26	21.76
RE	8.79	8.23	7.57	6.83	6.08	5.37	5.00	4.68	4.34	3.99	3.69	3.43
t	21.54	21.58	21.63	21.71	21.83	22.01	26.81	27.01	27.33	27.84	28.70	30.22
RS	88.18	82.59	75.87	68.43	60.85	53.71	44.81	41.93	38.77	35.61	32.72	30.23
IS	1.99	2.12	2.31	2.56	2.88	3.26	3.22	3.43	3.68	3.97	4.24	4.44

474	C9H9I2NO3		I2-Tyr					-21.0 -42.0		6.500 9.690	433.0	
No.	32	33	34	35	36	37	38	39	40	41	42	43
pHL	6.40	6.60	6.80	7.00	7.20	7.40	7.40	7.60	7.80	8.00	8.20	8.40
pHS	7.04	7.13	7.26	7.41	7.58	7.76	7.74	7.90	8.08	8.27	8.46	8.65
mS	14.97	15.62	16.33	17.02	17.62	18.13	17.91	18.27	18.64	19.05	19.54	20.19
RE	4.99	4.78	4.57	4.39	4.24	4.12	4.17	4.09	4.01	3.92	3.82	3.70
t	34.91	34.95	35.01	35.08	35.17	35.29	23.92	24.05	24.25	24.56	25.01	25.64
RS	42.08	40.34	38.59	37.02	35.75	34.76	42.88	42.02	41.18	40.30	39.27	38.00
IS	3.60	3.76	3.93	4.11	4.27	4.40	5.32	5.44	5.57	5.71	5.89	6.13

No.	44	45	46	47	48	49	50	51	52	53	54	55
pHL	8.20	8.40	8.60	8.80	9.00	9.20	9.00	9.20	9.40	9.60	9.80	10.00
pHS	8.53	8.71	8.89	9.07	9.25	9.43	9.36	9.51	9.67	9.84	10.02	10.21
mS	19.77	20.44	21.33	22.46	23.85	25.43	24.95	26.35	27.86	29.37	30.77	31.98
RE	3.78	3.65	3.50	3.33	3.13	2.94	2.99	2.83	2.68	2.54	2.43	2.33
t	26.47	27.13	27.98	29.02	30.22	31.46	37.44	38.56	39.69	40.94	42.32	44.06
RS	37.91	36.66	35.12	33.33	31.36	29.37	26.86	25.39	23.97	22.67	21.53	20.57
IS	5.81	6.05	6.38	6.79	7.29	7.85	7.03	7.51	8.04	8.54	8.96	9.25

EXAMPLE OF APPLICATION

Fig. 1 shows the pH dependence of the effective mobility of polyglycines, butyric acid and carbonic acid at infinite dilution (ionic strength = 0) The curves were plotted using the values shown in Table V. The curves are useful for the assessment of separability to a first approximation.

Fig. 2. shows the simulated R_E *vs.* pH_L curves. The values were taken from Table V. It was expected from Fig. 2 that the separation of these samples might be possible in the pH range 8.3–9 (pH buffer = Tris or amediol).

Fig. 3 shows the simulated and the observed isotachopherograms at pH 8.4 (pH buffer = Tris). Carbonic acid was contained in the terminating electrolyte. Good agreement was obtained, suggesting the utility of the simulation.

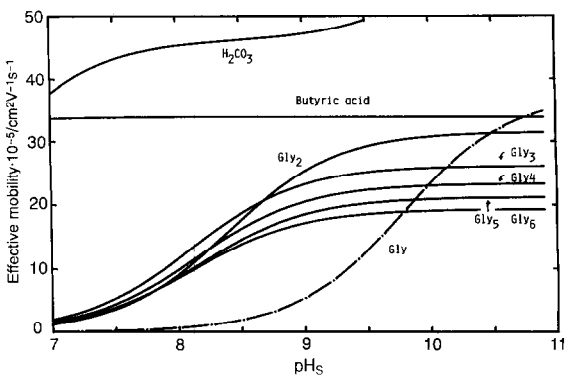

Fig. 1. pH dependence of the effective mobilities of carbonic acid (H_2CO_3), butyric acid, diglycine (Gly_2), triglycine (Gly_3), tetraglycine (Gly_4), pentaglycine (Gly_5), hexaglycine (Gly_6) and glycine (Gly). The curves are not for the isotachophoretic steady state. pH_S = pH of samples.

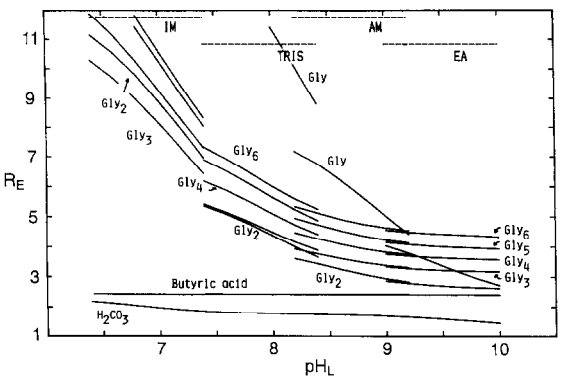

Fig. 2. pH dependence of the R_E values simulated for the samples shown in Fig. 1. pH buffers: IM = imidazole; Tris = tris(hydroxymethyl)aminomethane (Tris); AM = amediol; EA = ethanolamine.

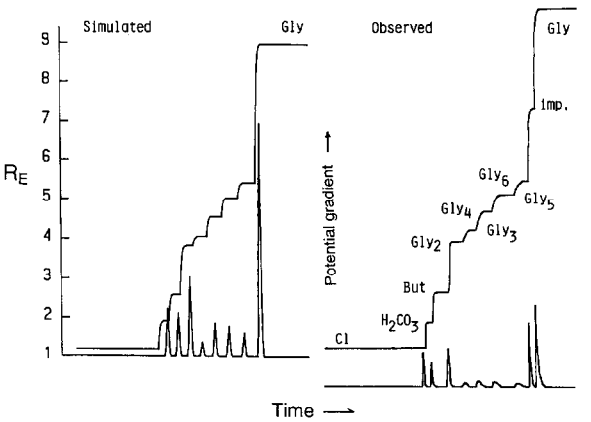

Fig. 3. Simulated and observed isotachopherograms for the samples in Figs. 1 and 2 at pH_L = 8.4 (Tris buffer). The terminator was glycine. The leading electrolyte contained 0.1% of hydroxypropylcellulose.

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