

APPENDIX: MATHEMATICAL MODELLING, STATISTICS AND NOMENCLATURE

Mathematical modelling of nutritional processes

Papers in which mathematical modelling of nutritional processes forms the principal element will be considered for publication provided: (a) they are based on sound biological and mathematical principles; (b) they advance nutritional concepts or identify new avenues likely to lead to such advances; (c) assumptions used in their construction are fully described and supported by appropriate argument; (d) they are described in such a way that the nutritional purpose is clearly apparent; (e) the contribution of the model to the design of future experimentation is clearly defined.

Units

Results should be presented in metric units according to the International System of Units (see Quantities, Units and Symbols in Physical Chemistry, 3rd ed. (2007) Cambridge: RSC Publishing), and Metric Units, Conversion Factors and Nomenclature in Nutritional and Food Sciences (1972) London: The Royal Society – as reproduced in *Proceedings of the Nutrition Society* (1972) **31**, 239–247). SI units should be used throughout the paper. The author will be asked to convert any values that are given in any other form. The only exception is where there is a unique way of expressing a particular variable that is in widespread use. Energy values must be given in Joules (MJ or kJ) using the conversion factor 1 kcal = 4.184 kJ. If required by the author, the value in kcal can be given afterwards in parentheses. Temperature is given in degrees Celsius (°C). Vitamins should be given as mg or µg, not as IU.

For substances of known molecular mass (Da) or relative molecular mass, e.g. glucose, urea, Ca, Na, Fe, K, P, values should be expressed as mol/l; for substances of indeterminate molecular mass (Da) or relative molecular mass, e.g. phospholipids, proteins, and for trace elements, e.g. Cu, Zn, then g/l should be used.

The 24 h clock should be used, e.g. 15.00 hours.

Units are: year, month, week, d, h, min, s, kg, g, mg, µg, litre, ml, µl, fl. To avoid misunderstandings, the word litre should be used in full, except in terms like g/l. Radioactivity should be given in becquerels (Bq or GBq) not in Ci. 1 MBq = 27.03 µCi (1Bq = 1 disintegration/s).

Statistical treatment of results

Data from individual replicates should not be given for large experiments, but may be given for small studies. The methods of statistical analysis used should be described, and references to statistical analysis packages included in the text, thus: Statistical Analysis Systems statistical software package version 6.11 (SAS Institute, Cary, NC, USA). Information such as analysis of variance tables should be given in the paper only if they are relevant to the discussion. A statement of the number of replicates, their average value and some appropriate measure of variability is usually sufficient.

Comparisons between means can be made by using either confidence intervals (CI) or significance tests. The most appropriate of such measures is usually the standard error of a difference between means (SED), or the standard errors of the means (SE or SEM) when these vary between means. The standard deviation (SD) is more useful only when there is specific interest in the variability of individual values. The degrees of freedom (df) associated with SED, SEM or SD should also be stated. The number of decimal places quoted should be sufficient but not excessive. Note that pH is an exponential number, as are the log(10) values often quoted for microbial numbers. Statistics should be carried out on the scalar rather than the exponential values.

If comparisons between means are made using CI, the format for presentation is, e.g. 'difference between means 0.73 (95 % CI 0.314, 1.36) g'. If significance tests are used, a statement that the difference between the means for two groups of values is (or is not) statistically significant should include the level of significance attained, preferably as an explicit P value (e.g. P=0.016 or P=0.32) rather than as a range (e.g. P<0.05 or P>0.05). It should be stated whether the significance levels quoted are one-sided or two-sided. Where a multiple comparison procedure is used, a description or explicit reference should be given. Where appropriate, a superscript notation may be used in tables to denote levels of significance; similar superscripts should denote lack of a significant difference.

Where the method of analysis is unusual, or if the experimental design is at all complex, further details (e.g. experimental plan, raw data, confirmation of assumptions, analysis of variance tables, etc.) should be included.

Chemical formulas

These should be written as far as possible on a single horizontal line. With inorganic substances, formulas may be used from first mention. With salts, it must be stated whether or not the anhydrous material is used, e.g. anhydrous CuSO_4 , or which of the different crystalline forms is meant, e.g. $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$, $\text{CuSO}_4 \cdot \text{H}_2\text{O}$.

Descriptions of solutions, compositions and concentrations

Solutions of common acids, bases and salts should be defined in terms of molarity (M), e.g. 0.1 M- NaH_2PO_4 . Compositions expressed as mass per unit mass (w/w) should have values expressed as ng, μg , mg or g per kg; similarly for concentrations expressed as mass per unit volume (w/v), the denominator being the litre. If concentrations or compositions are expressed as a percentage, the basis for the composition should be specified (e.g. % (w/w) or % (w/v) etc.). The common measurements used in nutritional studies, e.g. digestibility, biological value and net protein utilization, should be expressed as decimals rather than as percentages, so that amounts of available nutrients can be obtained from analytical results by direct multiplication. See *Metric Units, Conversion Factors and Nomenclature in Nutritional and Food Sciences*. London: The Royal Society, 1972 (para. 8).

Gene nomenclature and symbols

The use of symbols and nomenclature recommended by the [HUGO Gene Nomenclature Committee](#) is encouraged. Information on human genes is also available from [Entrez Gene](#), on mouse genes from the [Mouse Genome Database](#) and on rat genes from the [Rat Genome Database](#).

Nomenclature of vitamins

Most of the names for vitamins and related compounds that are accepted by the Editors are those recommended by the IUNS Committee on Nomenclature. See *Nutrition Abstracts and Reviews* (1978) **48A**, 831–835.

Acceptable name	Other names*
<i>Vitamin A</i>	
Retinol	Vitamin A ₁
Retinaldehyde, retinal	Retinene
Retinoic acid (all-trans or 13-cis)	Vitamin A ₁ acid
3-Dehydroretinol	Vitamin A ₂
<i>Vitamin D</i>	
Ergocalciferol, ercalciol	Vitamin D ₂ calciferol
Cholecalciferol, calciol	Vitamin D ₃
<i>Vitamin E</i>	
α -, β - and γ -tocopherols plus tocotrienols	
<i>Vitamin K</i>	
Phylloquinone	Vitamin K ₁
Menaquinone-n (MK-n)†	Vitamin K ₂
Menadione	Vitamin K ₃ , menaquinone, menaphthone
<i>Vitamin B₁</i>	
Thiamin	Aneurin(e), thiamine
<i>Vitamin B₂</i>	
Riboflavin	Vitamin G, riboflavine, lactoflavin
<i>Niacin</i>	
Nicotinamide	Vitamin PP
Nicotinic acid	
<i>Folic Acid</i>	

Pteroyl(mono)glutamic acid <i>Vitamin B₆</i>	Folacin, vitamin B ₉ or M
Pyridoxine Pyridoxal Pyridoxamine <i>Vitamin B₁₂</i>	Pyridoxol
Cyanocobalamin Hydroxocobalamin Aquocobalamin Methylcobalamin Adenosylcobalamin <i>Inositol</i>	Vitamin B _{12a} or B _{12b}
<i>Myo</i> -inositol <i>Choline</i>	<i>Meso</i> -inositol
<i>Pantothenic acid</i> <i>Biotin</i> <i>Vitamin C</i>	Vitamin H
Ascorbic acid Dehydroascorbic acid	

*Including some names that are still in use elsewhere, but are not used by the journal.

†Details of the nomenclature for these and other naturally-occurring quinones should follow the Tentative Rules of the IUPAC-IUB Commission on Biochemical Nomenclature (see *European Journal of Biochemistry* (1975) **53**, 15–18).

The terms **vitamin A**, **vitamin C** and **vitamin D** may still be used where appropriate, for example in phrases such as 'vitamin A deficiency', 'vitamin D activity'.

Values for vitamin D should be retrospectively or prospectively standardized, as recommended by *Sempos CT, Binkley N (2020). 25-Hydroxyvitamin D assay standardisation and vitamin D guidelines paralysis. Public Health Nutr 23, 1153-1164. DOI: 10.1017/S1368980019005251*. Authors of experimental or clinical studies for which such standardised data are not available must provide clear justification for their choice of assay.

The term **vitamin E** should be used as the descriptor for all tocol and tocotrienol derivatives exhibiting qualitatively the biological activity of α -tocopherol. The term **tocopherols** should be used as the generic descriptor for all methyl tocols. Thus, the term **tocopherol** is not synonymous with the term **vitamin E**.

The term **vitamin K** should be used as the generic descriptor for 2-methyl-1,4-naphthoquinone (menaphthone) and all derivatives exhibiting qualitatively the biological activity of phyloquinone (phytylmenaquinone).

The term **niacin** should be used as the generic descriptor for pyridine 3-carboxylic acid and derivatives exhibiting qualitatively the biological activity of nicotinamide.

The term **vitamin B₆** should be used as the generic descriptor for all 2-methylpyridine derivatives exhibiting qualitatively the biological activity of pyridoxine.

Regarding **folate**, due to the wide range of C-substituted, unsubstituted, oxidized, reduced and mono- or polyglutamyl side-chain derivatives of pteroylmonoglutamic acid that exist in nature, it is not possible to provide a complete list. Authors are encouraged to use either the generic name or the correct scientific name(s) of the derivative(s), as appropriate for each circumstance.

The term **vitamin B₁₂** should be used as the generic descriptor for all corrinoids exhibiting qualitatively the biological activity of cyanocobalamin. The term **corrinoids** should be used as the generic descriptor for all compounds containing the corrin nucleus and thus chemically related to cyanocobalamin. The term **corrinoid** is not synonymous with the term **vitamin B₁₂**.

The terms **ascorbic acid** and **dehydroascorbic acid** will normally be taken as referring to the naturally occurring L-forms. If the subject matter includes other optical isomers, authors are encouraged to include the L- or D- prefixes, as appropriate. The same is true for all those vitamins which can exist in both natural and alternative isomeric forms.

Weight units are acceptable for the amounts of vitamins in foods and diets. For concentrations in biological tissues, SI units should be used; however, the authors may, if they wish, also include other units, such as weights or international units, in parentheses. See *Metric Units, Conversion Factors and Nomenclature in Nutritional and Food Sciences* (1972) paras 8 and 14–20. London: The Royal Society.

Nomenclature of fatty acids and lipids

In the description of results obtained for the analysis of fatty acids by conventional GLC, the shorthand designation proposed by Farquhar JW, Insull W, Rosen P, Stoffel W & Ahrens EH (*Nutrition Reviews* (1959), 17, Suppl.) for individual fatty acids should be used in the text, tables and figures. Thus, 18 : 1 should be used to represent a fatty acid with eighteen carbon atoms and one double bond; if the position and configuration of the double bond is unknown. The shorthand designation should also be used in the abstract. If the positions and configurations of the double bonds are known, and these are important to the discussion, then a fatty acid such as linoleic acid may be referred to as *cis*-9,*cis*-12-18 : 2 (positions of double bonds related to the carboxyl carbon atom 1). However, to illustrate the metabolic relationship between different unsaturated fatty acid families, it is sometimes more helpful to number the double bonds in relation to the terminal methyl carbon atom, *n*. The preferred nomenclature is then: 18 : 3*n*-3 and 18 : 3*n*-6 for α -linolenic and γ -linolenic acids respectively; 18 : 2*n*-6 and 20 : 4*n*-6 for linoleic and arachidonic acids respectively and 18 : 1*n*-9 for oleic acid. Positional isomers such as α - and γ -linolenic acid should always be clearly distinguished. It is assumed that the double bonds are methylene-interrupted and are of the *cis*-configuration (see Holman RT in *Progress in the Chemistry of Fats and Other Lipids* (1966) vol. 9, part 1, p. 3. Oxford: Pergamon Press). Groups of fatty acids that have a common chain length but vary in their double bond content or double bond position should be referred to, for example, as C₂₀ fatty acids or C₂₀ PUFA. The modern nomenclature for glycerol esters should be used, i.e. triacylglycerol, diacylglycerol, monoacylglycerol *not* triglyceride, diglyceride, monoglyceride. The form of fatty acids used in diets should be clearly stated, i.e. whether ethyl esters, natural or refined fats or oils. The composition of the fatty acids in the dietary fat and tissue fats should be stated clearly, expressed as mol/100 mol or g/100 g total fatty acids.

Nomenclature of micro-organisms

The correct name of the organism, conforming with international rules of nomenclature, should be used. If desired, synonyms may be added in parentheses when the name is first mentioned. Names of bacteria should conform to the current Bacteriological Code and the opinions issued by the International Committee on Systematic Bacteriology. Names of algae and fungi must conform to the current International Code of Botanical Nomenclature. Names of protozoa should conform to the current International Code of Zoological Nomenclature.

Nomenclature of plants

For plant species where a common name is used that may not be universally intelligible, the Latin name in italics should follow the first mention of the common name. The cultivar should be given where appropriate.

Other nomenclature, symbols and abbreviations

Authors should consult recent issues of the journal for guidance. The IUPAC rules on chemical nomenclature should be followed, and the recommendations of the Nomenclature Committee of IUBMB and the IUPACIUBMB Joint Commission on Biochemical Nomenclature and Nomenclature Commission of IUBMB in *Biochemical Nomenclature and Related Documents* (1992), 2nd ed., London: Portland Press (<http://www.chem.qmul.ac.uk/iupac/bibliog/white.html>). The symbols and abbreviations, other than units, are essentially those listed in *British Standard 5775* (1979–1982), *Specifications for Quantities, Units and Symbols*, parts 0–13. Day should be abbreviated to d, for example 7 d, except for 'each day', '7th day' and 'day 1'.

Elements and simple chemicals (e.g. Fe and CO₂) can be referred to by their chemical symbol (with the exception of arsenic and iodine, which should be written in full) or formula from the first mention in the text; the title, text and table headings, and figure legends can be taken as exceptions. Well-known abbreviations for chemical substances may be used without explanation, thus: RNA for ribonucleic acid and DNA for deoxyribonucleic acid. Other substances that are mentioned frequently (five or more times) may also be abbreviated, the abbreviation being placed in parentheses at the first mention, thus: lipoprotein lipase (LPL), after that, LPL, and an alphabetical list of abbreviations used should be included. Only accepted abbreviations

may be used in the title and text headings. If an author's initials are mentioned in the text, they should be distinguished from other abbreviations by the use of stops, e.g. 'one of us (P. J. H.)...'. For UK counties the official names given in the *Concise Oxford Dictionary* (1995) should be used and for states of the USA two-letter abbreviations should be used, e.g. MA (not Mass.) and IL (not Ill.). Terms such as 'bioavailability' or 'available' may be used providing that the use of the term is adequately defined.

Spectrophotometric terms and symbols are those proposed in *IUPAC Manual of Symbols and Terminology for Physicochemical Quantities and Units* (1979) London: Butterworths. The attention of authors is particularly drawn to the following symbols: m (milli, 10^3), μ (micro, 10^6), n (nano, 10^9) and p (pico, 10^{12}). Note also that ml (millilitre) should be used instead of cc, μm (micrometre) instead of μ (micron) and μg (microgram) instead of γ .

Numerals should be used with units, for example, 10 g, 7 d, 4 years (except when beginning a sentence, thus: 'Four years ago...'); otherwise, words (except when 100 or more), thus: one man, ten ewes, ninety-nine flasks, three times (but with decimal, 2.5 times), 100 patients, 120 cows, 136 samples.

Abbreviations

The following abbreviations are accepted without definition by the journal:

ADP (GDP)	adenosine (guanosine) 5'-disphosphate
AIDS	acquired immune deficiency syndrome
AMP (GMP)	adenosine (guanosine) 5'-monophosphate
ANCOVA	analysis of covariance
ANOVA	analysis of variance
apo	apolipoprotein
ATP (GTP)	adenosine (guanosine) 5'-triphosphate
AUC	area under the curve
BMI	body mass index
BMR	basal metabolic rate
bp	base pair
BSE	bovine spongiform encephalopathy
CHD	coronary heart disease
CI	confidence interval
CJD	Creutzfeldt-Jacob disease
CoA and acyl-CoA	co-enzyme A and its acyl derivatives
CV	coefficient of variation
CVD	cardiovascular disease
Df	degrees of freedom
DHA	docosahexaenoic acid
DM	dry matter
DNA	deoxyribonucleic acid
dpm	disintegrations per minute
EDTA	ethylenediaminetetra-acetic acid
ELISA	enzyme-linked immunosorbent assay
EPA	eicosapentaenoic acid
Expt	experiment (for specified experiment, e.g. Expt 1)
FAD	flavin-adenine dinucleotide
FAO	Food and Agriculture Organization (except when used as an author)
FFQ	food-frequency questionnaire
FMN	flavin mononucleotide
GC	gas chromatography
GLC	gas-liquid chromatography
GLUT	glucose transporter
GM	genetically modified
Hb	haemoglobin
HDL	high-density lipoprotein
HEPES	4-(2-hydroxyethyl)-1-piperazine-ethanesulfonic acid
HIV	human immunodeficiency virus

HPLC	high-performance liquid chromatography
Ig	immunoglobulin
IHD	ischaemic heart disease
IL	interleukin
IR	infra red
Kb	kilobases
K_m	Michaelis constant
LDL	low-density lipoprotein
MHC	major histocompatibility complex
MRI	magnetic resonance imaging
MS	mass spectrometry
MUFA	monounsaturated fatty acids
NAD ⁺ , NADH	oxidized and reduced nicotinamide-adenine dinucleotide
NADP ⁺ , NADPH	oxidized and reduced nicotinamide-adenine dinucleotide phosphate
NEFA	non-esterified fatty acids
NF- κ B	nuclear factor kappa B
NMR	nuclear magnetic resonance
NS	not significant
NSP	non-starch polysaccharide
OR	odds ratio
PAGE	polyacrylamide gel electrophoresis
PBS	phosphate-buffered saline
PCR	polymerase chain reaction
PG	prostaglandin
PPAR	peroxisome proliferator-activated receptor
PUFA	polyunsaturated fatty acids
RDA	recommended dietary allowance
RER	respiratory exchange ratio
RIA	radioimmunoassay
RMR	resting metabolic rate
RNA, mRNA etc.	ribonucleic acid, messenger RNA etc.
rpm	revolutions per minute
RT	reverse transcriptase
SCFA	short-chain fatty acids
SDS	sodium dodecyl sulphate
SED	standard error of the difference between means
SFA	saturated fatty acids
SNP	single nucleotide polymorphism
TAG	triacylglycerol
TCA	trichloroacetic acid
TLC	thin-layer chromatography
TNF	tumour necrosis factor
UN	United Nations (except when used as an author)
UNICEF	United Nations International Children's Emergency Fund
UV	ultra violet
VLDL	very-low-density lipoprotein
V_{O_2}	O_2 consumption
V_{O_2max}	maximum O_2 consumption
WHO	World Health Organization (except when used as an author)
Use of three-letter versions of amino acids in tables: Leu, His, etc.	
CTP, UTP, GTP, ITP, as we already use ATP, AMP etc.	

Disallowed words and phrases

The following are disallowed by the journal: deuterium or tritium (use 2H and 3H)
c.a. or around (use approximately or about) canola (use rapeseed) ether (use diethyl ether) free fatty acids (use NEFA)

isocaloric/calorie (use isoenergetic/energy) quantitate
(use quantify)
unpublished data or observations (use unpublished results)