Thermodynamics of Enzyme-Catalyzed Reactions: Part 7—2007 Update

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This review serves to update previously published evaluations of equilibrium constants and enthalpy changes for enzyme-catalyzed reactions. For each reaction, the following information is given: the reference for the data, the reaction studied, the name of the enzyme used and its Enzyme Commission number, the method of measurement, the conditions of measurement [temperature, pH, ionic strength, and the buffer(s) and cofactor(s) used], the data and their evaluation, and, sometimes, commentary on the data and on any corrections which have been applied to the data or any calculations for which the data have been used. The review contains data from 119 references which have been examined and evaluated. Chemical Abstract Service registry numbers are given for the substances involved in these various reactions. There is also a cross reference between the substances and the Enzyme Commission numbers of the enzymes used to catalyze the reactions in which the substances participate. *© 2007 by the U.S. Secretary of Commerce on behalf of the United States. All rights reserved.* [DOI: 10.1063/1.2789450]

Key words: apparent equilibrium constants; enthalpies of reaction; enzyme-catalyzed reactions; evaluated data; transformed thermodynamic properties.

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1. Introduction

This paper serves to update a series of reviews[1–6] on the thermodynamics of enzyme-catalyzed reactions. These reviews, which were published during the years 1993–1999, deal with the thermodynamics of the reactions catalyzed by the six classes of enzymes classified by the Nomenclature Committee of the International Union of Biochemistry:[7] oxidoreductases,[1] transferases,[2] hydrolases,[3] lyases,[4] isomerases,[5] and ligases.[5] The first update[6] was published in 1999. The current review updates these earlier publications by providing coverage of the literature through the end of February 2007. Thus, while the current update primarily consists of papers published since the completion of the earlier reviews,[1–6] additional papers which contain data missed previously are also included. Accordingly, it is important that anyone examining a given reaction for which data are given in this review also consult the earlier reviews[1–6] in order to determine if more reliable results have been published previously.

Enzyme-catalyzed reactions play significant roles in many biological processes such as glycolysis, the anabolism and catabolism of carbohydrates, and fermentation and physiological processes such as vision. Many of these reactions are also of current or potential importance for the production of pharmaceuticals, biofuels, and bulk commodity chemicals such as ethanol, fructose, and amino acids. The data presented herein are limited to equilibrium and calorimetric measurements performed on these reactions under *in vitro* conditions. Thus, the thermodynamic quantities which are generally given are apparent equilibrium constants K' and calorimetrically determined enthalpies of reaction $\Delta_r H$(cal). Apparent equilibrium constants calculated from kinetic measurements (Haldane relations) are also tabulated. If the change in binding of hydrogen ion $\Delta_r N(H^+)$ in a biochemical reaction and the enthalpy of protonation of the buffer are known, the standard molar transformed enthalpy of reaction $\Delta_r H'^\circ$ can be calculated from the calorimetrically determined enthalpy of reaction.[8] Equilibrium constants K and standard molar enthalpies of reaction $\Delta_r H^\circ$ for chemical reference reactions are also given if they have been reported in the literature. The standard molar transformed enthalpy of reaction $\Delta_r H'^\circ$ can be used to calculate the temperature dependence of apparent equilibrium constants K' in the same way that the standard molar enthalpy of reaction $\Delta_r H^\circ$ is used to calculate the temperature dependence of the equilibrium constant K.

These data also serve as a basis for many additional thermodynamic calculations. Thus, Alberty[9–11] has used data given in the previous reviews[1–6] to calculate tables of standard molar transformed formation properties that are useful for the calculation of apparent equilibrium constants K' and standard molar transformed enthalpies of reaction $\Delta_r H'^\circ$ under specified conditions of temperature, pH, pMg, and ionic strength. If the prerequisite thermodynamic quantities on the binding of H^+(aq) and metal ions are available, it is also possible to calculate standard thermodynamic quantities (K and $\Delta_r H^\circ$) for reference reactions that involve specific species. Such calculations serve to transform the results of measurements made under varied conditions and that pertain to a mixture of species to results for reference reactions that pertain to the same standard state. Thus, once a sufficiently large reaction catalog has been established, thermodynamic network calculations[12] can be performed both to check the consistency of the data and to calculate "best" values of standard molar formation properties. Finally, and most importantly, these standard molar formation properties can then be used to calculate values of K and $\Delta_r H^\circ$ for a very large number of reactions that have not been the subject of investigation.

A good introduction to the thermodynamic principles involved in these studies can be found in IUPAC-IUBMB Recommendations.[13] On a more advanced level, two excellent books that deal with the thermodynamic principles underlying these studies are *Thermodynamics of Biochemical Reactions*[14] and *Biochemical Thermodynamics: Applications of Mathematica*.[15] The latter book contains several computer programs that are very useful for performing thermodynamic calculations on biochemical reactions. A Mathematica program[16] that can be used to calculate a wide variety of thermodynamic quantities [e.g., values of K and $\Delta_r H^\circ$ from measured values of K' and $\Delta_r H$(cal), values of K' as a function of temperature, pH, ionic strength, etc.] has also been published in the *Mathematica Journal*.

The data in this review are presented in the same format as in the previous reviews.[1–6] Thus, the following information is given for each entry in this review: the reference for the

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data, the biochemical reaction studied, the name of the enzyme used and its Enzyme Commission number, the method of measurement, the conditions of measurement [temperature, pH, ionic strength, and the buffer(s) and cofactor(s) used], the data and their evaluation, and, sometimes, commentary on the data and on any corrections which have been applied to the data or any calculations for which the data have been used. The absence of a piece of information indicates that it was not found in the paper cited. The arrangement of the data, their evaluation, and the thermodynamic conventions have been discussed previously.[1] In this regard, one should express equilibrium constants as dimensionless quantities. However, the numerical value obtained for the equilibrium constant of an unsymmetrical reaction will depend on the measure of composition and standard concentration selected for the reactants and products. Thus, for the chemical reaction

$$\mathrm{A(aq)} = \mathrm{B(aq)} + \mathrm{C(aq)}, \tag{1}$$

$K_c = c(\mathrm{B})c(\mathrm{C})/[c(\mathrm{A})c^\circ]$, $K_m = m(\mathrm{B})m(\mathrm{C})/[m(\mathrm{A})m^\circ]$, and $K_x = x(\mathrm{B})x(\mathrm{C})/x(\mathrm{A})$. Here, c, m, and x are, respectively, concentration, molality, and mole fraction, $c^\circ = 1$ mol dm^{-3}, and $m^\circ = 1$ mol kg^{-1}. The equilibrium constant expressed in terms of mole fractions is automatically dimensionless. Similar definitions and considerations apply to the apparent equilibrium constant K'. The symbols used in this review are given in the glossary (see Sec. 7).

The *subjective* evaluation of the data in this review consisted of the assignment of a rating: A (high quality), B (good), C (average), or D (low quality). In making these assignments, we considered the various experimental details which were provided in the study. These details include the method of measurement, the number of data points determined, and the extent to which the effects of varying temperature, pH, and ionic strength were investigated. A lower rating was generally given when few details of the investigation were reported. For example, in many of the papers cited, the major aim of the study was the isolation and purification of the enzyme of interest. Thus, the equilibrium data were obtained as only a small part of an investigation to characterize many of the properties of that enzyme and the reaction it catalyzes.

This effort began approximately 18 years ago with an extensive search of the literature to locate the papers containing the relevant data. This search was based on a carefully designed computer search of Chemical Abstracts, a manual search of Methods in Enzymology, and the examination of references found in earlier reviews that dealt with the thermodynamics of enzyme-catalyzed reactions.[17–27] The references obtained from these sources were in turn examined for additional references relevant to this effort. The current update, which covers the literature through the end of February 2007, relied primarily on a search of Chemical Abstracts and Medline. The authors would be most grateful if references that contain data on the thermodynamics of enzyme-catalyzed reactions that were not included in these reviews were brought to their attention.

Finally, the data published in these reviews are also available on the web as a NIST Standard Reference Database.[28,29] This database can be queried by using a variety of search terms.

2. Acknowledgments

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4. Table of Equilibrium Constants and Enthalpies of Reaction

4.1. Enzyme: alcohol dehydrogenase ($NADP^+$) (EC 1.1.1.2)

2-benzyl-1-cyclohexanone(sln) + 2-propanol(sln) = (±)-*cis*-2-benzyl-1-cyclohexanol(sln) + acetone(sln)

T/K	K
298.15	6.04

Reference: Tewari *et al.* (2007)[149]
Method: chromatography
Cofactor(s): NADP(red)
Evaluation: A

Here "sln" is *n*-hexane.

2-benzyl-1-cyclohexanone(sln) + 2-propanol(sln) = (±)-*trans*-2-benzyl-1-cyclohexanol(sln) + acetone(sln)

T/K	K
298.15	24.11

Reference: Tewari *et al.* (2007)[149]
Method: chromatography
Cofactor(s): NADP(red)
Evaluation: A

Here "sln" is *n*-hexane.

2-butanone(sln) + 2-propanol(sln) = (±)-2-butanol(sln) + acetone(sln)

T/K	Solvent	K
288.15	*n*-hexane	0.845
293.05	*n*-hexane	0.844
298.15	*n*-hexane	0.844
303.30	*n*-hexane	0.849
308.27	*n*-hexane	0.808
298.15	toluene	0.853
303.15	supercritical carbon dioxide (P=10.0 MPa)	0.820
298.15	methyl *tert*-butyl ether	0.814

Reference: Tewari *et al.* (2005)[134]
Method: chromatography
Cofactor(s): NADP(red)
Evaluation: A

Here "sln" is *n*-hexane, toluene, methyl *tert*-butyl ether, or supercritical carbon dioxide. Tewari *et al.* (2005)[134] calculated $\Delta_r G^\circ = 0.44$ kJ mol^{-1}, $\Delta_r H^\circ = -1.2$ kJ mol^{-1}, and $\Delta_r S^\circ = -5.5$ J K^{-1} mol^{-1} for this reaction carried out in *n*-hexane at T=298.15 K.

cyclobutanone(sln) + 2-propanol(sln) = cyclobutanol(sln) + acetone(sln)

T/K	Solvent	K
288.35	*n*-hexane	0.775
292.99	*n*-hexane	0.768
298.02	*n*-hexane	0.764
303.04	*n*-hexane	0.758
308.05	*n*-hexane	0.752
298.15	*n*-pentane	0.757
303.15	supercritical carbon dioxide (P=10.0 MPa)	0.722

Reference: Tewari *et al.* (2006)[144]
Method: chromatography
Cofactor(s): NADP(red)
Evaluation: A

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Here "sln" is *n*-hexane, *n*-pentane, or supercritical carbon dioxide. Tewari *et al.* (2006)[144] calculated $\Delta_r G^\circ = 0.670$ kJ mol^{-1}, $\Delta_r H^\circ = -1.09$ kJ mol^{-1}, and $\Delta_r S^\circ = -5.9$ J K^{-1} mol^{-1} for this reaction carried out in *n*-hexane at $T = 298.15$ K.

cycloheptanone(sln) + 2-propanol(sln) = cycloheptanol(sln) + acetone(sln)

T/K	Solvent	*K*
298.15	*n*-hexane	0.147
298.15	*n*-pentane	0.152

Reference: Tewari *et al.* (2006)[144]
Method: chromatography
Cofactor(s): NADP(red)
Evaluation: A

Here "sln" is *n*-hexane or *n*-pentane.

cyclohexanone(sln) + 2-propanol(sln) = cyclohexanol(sln) + acetone(sln)

T/K	Solvent	*K*
288.35	*n*-hexane	16.9
293.20	*n*-hexane	16.0
298.04	*n*-hexane	15.6
303.05	*n*-hexane	15.3
308.19	*n*-hexane	14.8
298.15	*n*-pentane	14.3
303.15	supercritical carbon dioxide ($P = 8.0$ MPa)	16.0
303.15	supercritical carbon dioxide ($P = 10.0$ MPa)	16.0
303.15	supercritical carbon dioxide ($P = 12.0$ MPa)	16.5

Reference: Tewari *et al.* (2006)[144]
Method: chromatography
Cofactor(s): NADP(red)
Evaluation: A

Here "sln" is *n*-hexane, *n*-pentane, or supercritical carbon dioxide. Tewari *et al.* (2006)[144] calculated $\Delta_r G^\circ = -6.82$ kJ mol^{-1}, $\Delta_r H^\circ = -4.6$ kJ mol^{-1}, and $\Delta_r S^\circ = 7.4$ J K^{-1} mol^{-1} for this reaction carried out in *n*-hexane at $T = 298.15$ K.

cyclooctanone(sln) + 2-propanol(sln) = cyclooctanol(sln) + acetone(sln)

T/K	Solvent	*K*
298.15	*n*-hexane	0.0314
298.15	*n*-pentane	0.0279

Reference: Tewari *et al.* (2006)[144]
Method: chromatography
Cofactor(s): NADP(red)
Evaluation: A

Here "sln" is *n*-hexane or *n*-pentane.

cyclopentanone(sln) + 2-propanol(sln) = cyclopentanol(sln) + acetone(sln)

T/K	Solvent	*K*
298.15	*n*-pentane	0.357
298.15	*n*-hexane	0.342
303.15	supercritical carbon dioxide ($P = 10.0$ MPa)	0.339

Reference: Tewari *et al.* (2006)[144]
Method: chromatography
Cofactor(s): NADP(red)
Evaluation: A

Here "sln" is *n*-hexane, *n*-pentane, or supercritical carbon dioxide.

2-heptanone(sln) + 2-propanol(sln) = (*S*)-2-heptanol(sln) + acetone(sln)

T/K	*K*
298.15	0.321

Reference: Tewari *et al.* (2005)[134]
Method: chromatography
Cofactor(s): NADP(red)
Evaluation: A

Here "sln" is *n*-hexane. The reported value $K = 0.338$ has been multiplied by 0.95 to account for the presence of a mole fraction $x = 0.05$ of the (*R*)-2-heptanol in the reaction mixture.

2-hexanone(sln) + 2-propanol(sln) = (±)-2-hexanol(sln) + acetone(sln)

T/K	*K*
298.15	0.459

Reference: Tewari *et al.* (2005)[134]
Method: chromatography
Cofactor(s): NADP(red)
Evaluation: A

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Here "sln" is *n*-hexane

2-methyl-1-cyclohexanone(sln)+2-propanol(sln)
=(±)-*cis*-2-methyl-1-cyclohexanol(sln)+acetone(sln)

T/K	K
288.15	2.21
293.15	2.36
298.15	2.22
303.15	1.97
308.15	1.93

Reference: Tewari *et al.* (2007)[149]
Method: chromatography
Cofactor(s): NADP(red)
Evaluation: A

Here "sln" is *n*-hexane. Tewari *et al.* (2007)[149] calculated $\Delta_r G^\circ = -1.87$ kJ mol^{-1}, $\Delta_r H^\circ = -6.56$ kJ mol^{-1}, and $\Delta_r S^\circ = -15.7$ J K^{-1} mol^{-1} for this reaction at $T = 298.15$ K.

2-methyl-1-cyclohexanone(sln)+2-propanol(sln)
=(±)-*trans*-2-methyl-1-cyclohexanol(sln)+acetone(sln)

T/K	K
288.15	11.17
293.15	11.11
298.15	10.05
303.15	10.55
308.15	10.53

Reference: Tewari *et al.* (2007)[149]
Method: chromatography
Cofactor(s): NADP(red)
Evaluation: A

Here "sln" is *n*-hexane. Tewari *et al.* (2007)[149] calculated $\Delta_r G^\circ = -5.87$ kJ mol^{-1}, $\Delta_r H^\circ = -2.54$ kJ mol^{-1}, and $\Delta_r S^\circ = 11.2$ J K^{-1} mol^{-1} for this reaction at $T = 298.15$ K.

2-octanone(sln)+2-propanol(sln)=(*S*)-(+)-2-octanol(sln)
+acetone(sln)

T/K	Solvent	K
298.15	*n*-hexane	0.313
298.15	toluene	0.311
298.15	methyl *tert*-butyl ether	0.313

Reference: Tewari *et al.* (2005)[134]
Method: chromatography
Cofactor(s): NADP(red)
Evaluation: A

Here "sln" is *n*-hexane, toluene, or methyl *tert*-butyl ether.

2-pentanone(sln)+2-propanol(sln)=(±)-2-pentanol(sln)
+acetone(sln)

T/K	Solvent	K
298.15	*n*-hexane	0.627
303.15	supercritical carbon dioxide (P=10.0 MPa)	0.634

Reference: Tewari *et al.* (2005)[134]
Method: chromatography
Cofactor(s): NADP(red)
Evaluation: A

Here "sln" is *n*-hexane or supercritical carbon dioxide.

1-phenyl-1-butanone(sln)+2-propanol(sln)
=(±)-1-phenyl-1-butanol(sln)+acetone(sln)

T/K	Solvent	K
298.15	*n*-hexane	0.2562
298.15	*n*-pentane	0.2648

Reference: Tewari *et al.* (2006)[143]
Method: chromatography
Cofactor(s): NADP(red)
Evaluation: A

Here "sln" is either *n*-hexane or *n*-pentane.

2-phenyl-1-cyclohexanone(sln)+2-propanol(sln)
=(±)-*cis*-2-phenyl-1-cyclohexanol(sln)+acetone(sln)

T/K	K
298.15	7.79

Reference: Tewari *et al.* (2007)[149]
Method: chromatography
Cofactor(s): NADP(red)
Evaluation: A

Here "sln" is *n*-hexane.

2-phenyl-1-cyclohexanone(sln)+2-propanol(sln)
=(±)-*trans*-2-phenyl-1-cyclohexanol(sln)+acetone(sln)

T/K	K
298.15	10.40

Reference: Tewari *et al.* (2007)[149]
Method: chromatography

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Cofactor(s): NADP(red)
Evaluation: A

Here "sln" is *n*-hexane.

1-phenyl-1-ethanone(sln)+2-propanol(sln)
=(±)-1-phenyl-1-ethanol(sln)+acetone(sln)

T/K	Solvent	K
288.36	*n*-hexane	0.2033
292.83	*n*-hexane	0.2132
297.93	*n*-hexane	0.2171
303.04	*n*-hexane	0.2227
308.05	*n*-hexane	0.2317
298.15	*n*-pentane	0.2089

Reference: Tewari *et al.* (2006)[143]
Method: chromatography
Cofactor(s): NADP(red)
Evaluation: A

Here "sln" is either *n*-hexane or *n*-pentane. Tewari *et al.* (2006)[143] calculated $\Delta_r G^\circ = 3.78$ kJ mol^{-1}, $\Delta_r H^\circ = 4.53$ kJ mol^{-1}, and $\Delta_r S^\circ = 2.5$ J K^{-1} mol^{-1} at $T = 298.15$ K for the above reaction carried out in *n*-hexane.

1-phenyl-1-heptanone(sln)+2-propanol(sln)
=(±)-1-phenyl-1-heptanol(sln)+acetone(sln)

T/K	Solvent	K
298.15	*n*-hexane	0.5697
298.15	*n*-pentane	0.5667

Reference: Tewari *et al.* (2006)[143]
Method: chromatography
Cofactor(s): NADP(red)
Evaluation: A

Here "sln" is either *n*-hexane or *n*-pentane.

1-phenyl-1-hexanone(sln)+2-propanol(sln)
=(±)-1-phenyl-1-hexanol(sln)+acetone(sln)

T/K	Solvent	K
298.15	*n*-hexane	0.3167
298.15	*n*-pentane	0.2976

Reference: Tewari *et al.* (2006)[143]
Method: chromatography
Cofactor(s): NADP(red)
Evaluation: A

Here "sln" is either *n*-hexane or *n*-pentane.

1-phenyl-1-pentanone(sln)+2-propanol(sln)
=(±)-1-phenyl-1-pentanol(sln)+acetone(sln)

T/K	Solvent	K
298.15	*n*-hexane	0.4797
298.15	*n*-pentane	0.4870

Reference: Tewari *et al.* (2006)[143]
Method: chromatography
Cofactor(s): NADP(red)
Evaluation: A

Here "sln" is either *n*-hexane or *n*-pentane.

1-phenyl-1-propanone(sln)+2-propanol(sln)
=(±)-1-phenyl-1-propanol(sln)+acetone(sln)

T/K	Solvent	K
298.15	*n*-hexane	0.3401
298.15	*n*-pentane	0.3626

Reference: Tewari *et al.* (2006)[143]
Method: chromatography
Cofactor(s): NADP(red)
Evaluation: A

Here "sln" is either *n*-hexane or *n*-pentane.

2-propanol(aq)+NADP(ox)(aq)=acetone(aq)
+NADP(red)(aq)

T/K	pH	I_c/(mol dm^{-3})	K'
278.15	5.88	0.25	0.001 45
278.15	6.32	0.25	0.003 70
278.15	6.80	0.25	0.0111
278.15	7.25	0.25	0.0277
278.15	7.62	0.25	0.0706
278.15	7.82	0.25	0.126
288.15	5.79	0.25	0.002 39
288.15	6.25	0.25	0.006 51
288.15	6.73	0.25	0.0169
288.15	7.18	0.25	0.0428
288.15	7.55	0.25	0.104
288.15	7.74	0.25	0.150
298.15	5.71	0.25	0.003 44
298.15	6.19	0.25	0.009 25
298.15	6.67	0.25	0.0260
298.15	7.11	0.25	0.0701
298.15	7.49	0.25	0.162
298.15	7.68	0.25	0.236
308.15	5.67	0.25	0.005 31
308.15	6.13	0.25	0.001 45
308.15	6.61	0.25	0.0425

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T/K	pH	I_c/(mol dm^{-3})	K'
308.15	7.06	0.25	0.113
308.15	7.43	0.25	0.251
308.15	7.62	0.25	0.393
313.15	5.63	0.25	0.005 33
313.15	6.10	0.25	0.001 45
313.15	6.58	0.25	0.0519
313.15	7.03	0.25	0.131
313.15	7.40	0.25	0.328
313.15	7.59	0.25	0.435
278.15	6.06	0.25	0.004 13
278.15	6.43	0.25	0.006 73
278.15	6.88	0.25	0.0183
278.15	7.38	0.25	0.0459
278.15	7.87	0.25	0.155
278.15	8.19	0.25	0.357
288.15	5.99	0.25	0.004 49
288.15	6.37	0.25	0.009 73
288.15	6.82	0.25	0.0236
288.15	7.31	0.25	0.0656
288.15	7.80	0.25	0.188
288.15	8.11	0.25	0.381
298.15	5.92	0.25	0.006 36
298.15	6.30	0.25	0.0132
298.15	6.75	0.25	0.0353
298.15	7.25	0.25	0.0967
298.15	7.72	0.25	0.292
298.15	8.02	0.25	0.551
308.15	5.87	0.25	0.009 38
308.15	6.25	0.25	0.0208
308.15	6.70	0.25	0.0558
308.15	7.19	0.25	0.144
308.15	7.66	0.25	0.477
308.15	7.96	0.25	0.882
313.15	5.85	0.25	0.0103
313.15	6.23	0.25	0.0233
313.15	6.69	0.25	0.0646
313.15	7.18	0.25	0.191
313.15	7.65	0.25	0.579
313.15	7.93	0.25	1.08

Reference: King (2003)[121]
Method: spectrophotometry coupled with enzymatic assay
Buffer: phosphate
pH: 5.63–8.19
Evaluation: A

King (2003)[121] used his results to calculate $K=5.98\cdot10^{-10}$, $\Delta_rG^\circ=52.65$ kJ mol^{-1}, $\Delta_rH^\circ=38.9$ kJ mol^{-1}, and $\Delta_rS^\circ=-46.1$ J K^{-1} mol^{-1} for the chemical reference reaction [2-propanol(aq)+NADP^{3-}(ox)(aq)=acetone(aq)+NADP^{4-}(red)(aq)+H$^+$(aq)] at $T=298.15$ K and $I=0$.

4.2. Enzyme: homoserine dehydrogenase (EC 1.1.1.3)

L-homoserine(aq)+NADP(ox)(aq)
=L-aspartate 4-semialdehyde(aq)+NADP(red)(aq)

T/K	pH	K'
310.15	9.0	0.010

Reference: Wedler *et al.*[70]
Method: spectrophotometry and radioactivity
Buffer: Ches (0.10 mol dm^{-3})
pH: 9.0
Evaluation: B

The same result was also given by Wedler and Ley (1993).[73]

4.3. Enzyme: mannitol-1-phosphate 5-dehydrogenase (EC 1.1.1.17)

D-mannitol-1-phosphate(aq)+NAD(ox)(aq)
=D-fructose 6-phosphate(aq)+NAD(red)(aq)

T/K	pH	K'
298.15	7.4	1.1
298.15	8.0	1.0

Reference: Zancan and Bacila (1964)[33]
Method: spectrophotometry
Buffer: glycylglycine (0.1 mol dm^{-3})
pH: 7.4–8.0
Evaluation: B

Zancan and Bacila reported $[K'c(H^+)]^{-1}=2.2\cdot10^7$ at pH=7.4 and $[K'c(H^+)]^{-1}=1.0\cdot10^8$ at pH=8.0. The values of K' given here were calculated from these results. The temperature was not reported but is assumed to be 298.15 K.

D-mannitol-1-phosphate(aq)+NAD(ox)(aq)
=D-fructose 6-phosphate(aq)+NAD(red)(aq)

T/K	pH	K'
298.15	9.0	0.79

Reference: Kiser and Niehaus (1981)[47]
Method: spectrophotometry
Buffer: Hepes
pH: 9.0
Evaluation: B

Kiser and Niehaus reported $K'c(H^+)=7.9\cdot10^{-10}$ at $T=298.15$ K and pH=9.0. The value of K' given here was calculated from this result.

4.4. Enzyme: D-lactate dehydrogenase (EC 1.1.1.28)

D-2-hydroxy-*n*-butanoate(aq)+NAD(ox)(aq)
=2-oxobutanoate(aq)+NAD(red)(aq)

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T/K	pH	K'
298.15	8.0	0.0028

Reference: Isobe *et al.* (2002)[115]
Method: spectrophotometry
Buffer: Tris (0.20 mol dm^{-3})+HCl
pH: 8.0
Evaluation: C

This result is based on kinetic data (Haldane relation) and is approximate.

(*R*)-lactate(aq)+NAD(ox)(aq)=pyruvate(aq)+NAD(red)(aq)

T/K	pH	K'
298.15	8.0	0.0037

Reference: Isobe *et al.* (2002)[115]
Method: spectrophotometry
Buffer: Tris (0.20 mol dm^{-3})+HCl
pH: 8.0
Evaluation: C

This result is based on kinetic data (Haldane relation) and is approximate.

4.5. Enzyme: malate dehydrogenase (EC 1.1.1.37)

(2*R*,3*R*)-*erythro*-fluoromalate(aq)+NAD(ox)(aq)=(3*R*)-fluorooxalacetate(aq)+NAD(red)(aq)

T/K	pH	K'
298.15	8.0	$6.3\cdot10^{-6}$

Reference: Urbauer *et al.* (1998)[85]
Method: spectrophotometry and electrochemistry
Buffer: Hepes (0.20 mol dm^{-3})+NaOH
pH: 8.00
Evaluation: A

Urbauer *et al.* reported $K'c(H^+)/c^\circ=6.3\cdot10^{-14}$ at pH=8.0. The value of the apparent equilibrium constant given here was calculated from this result.

(*S*)-malate(aq)+3-acetylpyridine adenine dinucleotide(ox)(aq)=oxaloacetate(aq)+3-acetylpyridine adenine dinucleotide(red)(aq)

T/K	pH	K'
298.15	8.0	$5.36\cdot10^{-3}$

Reference: Urbauer *et al.* (1998)[85]
Method: spectrophotometry
Buffer: Hepes (0.20 mol dm^{-3})+NaOH
pH: 8.00
Evaluation: A

Urbauer *et al.* reported $K'c(H^+)/c^\circ=5.36\cdot10^{-11}$ at pH=8.0. The value of the apparent equilibrium constant given here was calculated from this result.

(*S*)-malate(aq)+NAD(ox)(aq)=oxaloacetate(aq)+NAD(red)(aq)

T/K	pH	K'
298.15	8.0	$6.65\cdot10^{-5}$

Reference: Urbauer *et al.* (1998)[85]
Method: spectrophotometry
Buffer: Hepes (0.20 mol dm^{-3})+NaOH
pH: 8.00
Evaluation: A

Urbauer *et al.* reported $K'c(H^+)/c^\circ=6.65\cdot10^{-13}$ at pH=8.0. The value of the apparent equilibrium constant given here was calculated from this result.

4.6. Enzyme: pyridoxine 4-dehydrogenase (EC 1.1.1.65)

pyridoxine(aq)+NADP(ox)(aq)=pyridoxal(aq)+NADP(red)(aq)

T/K	pH	K'
298.15	6.0	$3.9\cdot10^{-6}$
298.15	9.0	$7.1\cdot10^{-3}$

Reference: Guirard and Snell (1988)[62]
Method: spectrophotometry
Buffer: citrate (0.060 mol dm^{-3}) and [Tris (0.060 mol dm^{-3})+HCl]
pH: 6.0–9.0
Cofactor(s): $MgCl_2$
Evaluation: B

Guirard and Snell reported $[K'c(H^+)]^{-1}=2.6\cdot10^{11}$ at pH=9.0 and $[K'c(H^+)]^{-1}=1.4\cdot10^{11}$ at pH=6.0. The values of the apparent equilibrium constants given here were calculated from these values.

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4.7. Enzyme: homoisocitrate dehydrogenase (EC 1.1.1.87)

3-carboxy-2-hydroxyadipate(aq)+NAD(ox)
=2-oxoadipate(aq)+carbon dioxide(aq)+NAD(red)

T/K	pH	K'_c
298.15	7.5	0.45

Reference: Lin *et al.* (2007)[147]
Method: spectrophotometry
Buffer: Hepes (0.050 mol dm^{-3})
pH: 7.5
Cofactor(s): $MgCl_2$ (0.010 mol dm^{-3})
Evaluation: A

A value of $K'=0.68$ ($T=298.15$ K, pH=7.5) was obtained by using the Haldane relation.

4.8. enzyme: dTDP-4-dehydrorhamnose reductase (EC 1.1.1.133)

dTDP-6-deoxy-**L**-lyxo-4-hexulose(aq)+NAD(red)(aq)
=dTDP-**L**-rhamnose(aq)+NAD(ox)(aq)

T/K	pH	K'
298.15	9.0	$3.6\cdot10^4$

Reference: Graninger *et al.* (1999)[89]
Method: chromatography
Buffer: ethanolamine (0.050 mol dm^{-3})+HCl
pH: 9.0
Cofactor(s): $MgCl_2$
Evaluation: B

Graninger *et al.* reported $[K'/c(H^+)]=3.6\cdot10^{13}$ at pH =9.0. The value of the apparent equilibrium constant given here was calculated from this value.

4.9. Enzyme: dTDP-4-dehydrorhamnose reductase (EC 1.1.1.133)

dTDP-6-deoxy-**D**-xylo-4-hexulose(aq)+NAD(red)(aq)
=dTDP-**L**-rhamnose(aq)+NAD(ox)(aq)

T/K	pH	K'
298.15	9.0	450

Reference: Graninger *et al.* (1999)[89]
Method: chromatography
Buffer: ethanolamine (0.050 mol dm^{-3})+HCl
pH: 9.0
Cofactor(s): $MgCl_2$
Evaluation: B

Graninger *et al.* reported $[K'/c(H^+)]=4.5\cdot10^{11}$ at pH =9.0. The value of the apparent equilibrium constant given here was calculated from this value. The enzyme dTDP-4-dehydrorhamnose 3,5-epimerase (EC 5.1.3.13) was also present.

4.10. Enzyme: 2-dehydropantoate 2-reductase (EC 1.1.1.169)

(*R*)-pantoate(aq)+NADP(ox)=2-dehydropantoate(aq)
+NADP(red)(aq)

T/K	pH	K'
298.15	7.5	0.001 48

Reference: Zheng and Blanchard (2000)[107]
Method: spectrophotometry
Buffer: Hepes (0.10 mol dm^{-3})
pH: 7.5
Evaluation: B

The value $K'=0.001\,02$ at $T=298.15$ K and pH=7.5 was obtained by using the Haldane relation.

4.11. Enzyme: 2,5-diketo-D-gluconate reductase (EC 1.1.1.274)

2-keto-**L**-gulonate(aq)+NADP(ox)(aq)
=2,5-diketo-**D**-gluconate(aq)+NADP(red)(aq)

T/K	pH	K'
298.15	9.2	0.000 89

Reference: Miller *et al.* (1987)[60]
Method: spectrophotometry
Buffer: [glycine (0.10 mol dm^{-3})+HCl] and sodium carbonate (0.040 mol dm^{-3})
pH: 9.2–9.6
Evaluation: C

Miller *et al.* reported $K'c(H^+)=5.6\cdot10^{-13}$ at $T=298.15$ K and over the pH range of 9.2–9.6. The values of K' given here were calculated from this result.

4.12. Enzyme: xanthine oxidase (EC 1.1.3.22)

xanthine(aq)+H_2O(l)+O_2(aq)=urate(aq)+H_2O_2(aq)

T/K	pH	Δ_rH(cal)/(kJ mol^{-1})
298.15	7.5	−5.25

Reference: Liang *et al.* (1998)[83]
Method: calorimetry
Buffer: phosphate
pH: 7.5
Evaluation: A

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4.13. Enzyme: succinate-semialdehyde reductase (EC 1.2.1.a)

4-oxobutanoate(aq)+NADP(red)(aq)
=4-hydroxybutanoate(aq)+NADP(ox)(aq)

T/K	pH	K'
298.15	7.0	3.7

Reference: Hearl and Churchich (1985)[55]
Method: spectrophotometry
Buffer: potassium phosphate (0.10 mol dm^{-3})
pH: 7.2
Evaluation: C

Hearl and Churchich reported $[K'/c(H^+)]=5.8\cdot10^7$ for pH=7.2. The apparent equilibrium constant given here was calculated from this value.

4.14. Enzyme: amine oxidase (copper-containing) (EC 1.4.3.6)

4-dimethylaminomethylbenzylamine(aq)+H_2O(1)
+O_2(aq)=4-dimethylaminomethylbenzaldehyde(aq)
+ammonia(aq)+H_2O_2(aq)

T/K	pH	I_c/(mol dm^{-3})	K'_c
298.15	7.15	0.22	2.7

Reference: Crabbe *et al.* (1976)[39]
Method: spectrophotometric and oxygen electrode
Buffer: phosphate
pH: 7.15
Evaluation: C

The reaction was carried out from only the forward direction of reaction. The temperature is assumed to be 298.15 K. The value of K' here was converted from the reported value $K'=2700$ based on millimolar concentrations.

4.15. Enzyme: dihydrofolate reductase (EC 1.5.1.3)

5,6,7,8-tetrahydrofolate(aq)+NADP(ox)(aq)
=7,8-dihydrofolate(aq)+NADP(red)(aq)

T/K	pH	K'
298.15	8.0	0.000 77
298.15	9.8	0.049

Reference: Fierke *et al.* (1987)[58]
Method: spectrophotometric
Buffer: Mes+Tris
pH: 8.0–9.8
Evaluation: B

Fierke *et al.* reported $[K'c(H^+)]^{-1}=1.3\cdot10^{11}$ for the range pH=8.0–9.8. The apparent equilibrium constants given here were calculated from this value.

4.16. Enzyme: methylenetetrahydrofolate dehydrogenase (NADP$^+$) (EC 1.5.1.5)

5,10-methylenetetrahydrofolate(aq)+NADP(ox)(aq)
=10-formyltetrahydrofolate(aq)+NADP(red)(aq)

T/K	pH	K'
303.15	7.3	16

Reference: Pelletier and MacKenzie (1995)[76]
Method: spectrophotometry and enzymatic assay
Buffer: potassium phosphate (0.025 mol dm^{-3})
pH: 7.3
Evaluation: B

4.17. Enzyme: saccharopine dehydrogenase (NAD$^+$, L-lysine forming) (EC 1.5.1.7)

N^6-(L-1,3-dicarboxypropyl)-L-lysine+NAD(ox)+H_2O(l)
=L-lysine(aq)+2-oxoglutarate(aq)+NAD(red)

T/K	pH	K'_c
298.15	7.0	$3.9\cdot10^{-7}$

Reference: Xu *et al.* (2006)[145]
Method: spectrophotometry
Buffer: Hepes (0.10 mol dm^{-3})
pH: 7.0
Evaluation: A

A value of $K'=2.9\cdot10^{-7}$ (T=298.15 K, pH=7.0) was obtained by using the Haldane relation.

4.18. Enzyme: NAD(P)$^+$ transhydrogenase (B-specific) (EC 1.6.1.1)

NAD(red)(aq)+NADP(ox)(aq)=NAD(aq)(ox)(aq)
+NADP(red)(aq)

T/K	pH	Buffer	c(KCl)/(mol dm^{-3})	I_c/(mol dm^{-3})	K'
298.15	7.60	Tris+HCl	0	0.0015	0.33
298.15	7.60	Tris+HCl	0.005	0.0061	0.35
298.15	7.60	Tris+HCl	0.010	0.0115	0.38
298.15	7.60	Tris+HCl	0.020	0.0216	0.43
298.15	7.60	Tris+HCl	0.050	0.0516	0.48
298.15	7.60	Tris+HCl	0.100	0.1014	0.54
298.15	6.11	phosphate	0	0.010	0.52
298.15	6.53	phosphate	0	0.010	0.44
298.15	6.99	phosphate	0	0.010	0.41
298.15	7.45	phosphate	0	0.010	0.38

Reference: Veeger and Krul (1977)[41]

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Method: spectrophotometry
Buffer: (Tris+HCl) and phosphate
pH: 6.11–7.60
Evaluation: A

4.19. Enzyme: glutathione reductase (NADPH) (EC 1.6.4.2)

2 glutathoine(red)(aq)+NADP(ox)(aq)= glutathoine(ox)(aq)+NADP(red)(aq)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_t H$(cal)/(kJ mol^{-1})
298.15	7.41	0.35	4.2

Reference: Tewari and Goldberg (2003)[125]
Method: chromatography and calorimetry
Buffer: phosphate
pH: 7.41
Evaluation: A

Tewari and Goldberg also calculated $K=6.5\cdot10^{-11}$, $\Delta_r G^\circ=58.1$ kJ mol^{-1}, $\Delta_r H^\circ=6.9$ kJ mol^{-1}, and $\Delta_r S^\circ=-172$ J K^{-1} mol^{-1} for the chemical reference reaction [2 glutathione(red)$^-$(aq)+NADP(ox)$^{3-}$(aq) =glutathione(ox)$^{2-}$(aq)+NADP(ox)$^{4-}$(aq)+H$^+$(aq)] at $T=298.15$ K and $I=0$.

2 glutathoine(red)(aq)+NADP(ox)(aq)= glutathoine(ox)(aq)+NADP(red)(aq)

T/K	pH	Buffer	Type of experiment	I_m (mol kg^{-1})	K'
298.15	6.66	phosphate	F	0.69	$6.9\cdot10^{-4}$
298.15	6.58	phosphate	EA	0.90	$4.6\cdot10^{-4}$
298.15	6.60	phosphate	SA	0.68	$7.0\cdot10^{-4}$
298.15	6.93	phosphate	F	0.67	$1.6\cdot10^{-3}$
298.15	6.85	phosphate	EA	0.73	$1.5\cdot10^{-3}$
298.15	6.90	phosphate	SA	0.67	$2.1\cdot10^{-3}$
298.15	8.23	Tris+HCl	F	0.091	0.0468
298.15	8.21	Tris+HCl	EA	0.091	0.0473
298.15	8.25	Tris+HCl	SA	0.091	0.0465
298.15	8.33	Tris+HCl	F	0.42	0.0432
298.15	8.34	Tris+HCl	EA	0.50	0.0410
298.15	8.34	Tris+HCl	SA	0.42	0.0487
298.15	8.61	Tris+HCl	F	0.48	0.0672
298.15	8.62	Tris+HCl	EA	0.71	0.0675
298.15	8.59	Tris+HCl	SA	0.47	0.0686
298.15	8.66	Tris+HCl	F	0.44	0.0452
298.15	8.68	Tris+HCl	EA	0.65	0.0466
298.15	8.67	Tris+HCl	SA	0.43	0.0489
298.15	8.47	Tris+HCl	F	0.32	0.0492
298.15	8.44	Tris+HCl	EA	0.59	0.0448
298.15	8.46	Tris+HCl	SA	0.31	0.0541
298.15	8.33	Tris+HCl	F	0.48	0.0494
298.15	8.35	Tris+HCl	EA	0.64	0.0511
298.15	8.38	Tris+HCl	SA	0.48	0.0508

Reference: Tewari and Goldberg (2003)[125]
Method: chromatography
Buffer: phosphate and Tris+HCl
pH: 7.41
Evaluation: A

In the table given here, "F," "EA," and "SA" refer to the three types of equilibrium measurements performed by Tewari and Goldberg: "F" is the measurement from the forward direction of reaction, "EA" is the experiment involving the addition of enzyme (glutathione reductase) to the reaction mixture, and "SA" is the experiment involving the addition of the additional substrate [glutathione(red)+NADP(ox)] to the reaction mixture. Tewari and Goldberg also calculated $K=6.5\cdot10^{-11}$, $\Delta_r G^\circ=58.1$ kJ mol^{-1}, $\Delta_r H^\circ=6.9$ kJ mol^{-1}, and $\Delta_r S^\circ=-172$ J K^{-1} mol^{-1} for the chemical reference reaction [2 glutathione(red)$^-$(aq)+NADP(ox)$^{3-}$(aq) =glutathione(ox)$^{2-}$(aq)+NADP(red)$^{4-}$(aq)+H$^+$(aq)] at $T=298.15$ K and $I=0$.

4.20. Enzyme: superoxide dismutase (EC 1.15.1.1)

$2O_2\cdot(aq)+2H^+(aq)=O_2(aq)+H_2O_2(aq)$

T/K	pH	$\frac{\Delta_t H^\circ}{\text{kJ mol}^{-1}}$
298.15	8.0	−160.1

Reference: Liang *et al.* (1998)[82]
Method: calorimetry
Buffer: sodium phosphate (0.05 mol dm^{-3})
pH: 8.0
Evaluation: B

Liang *et al.* used the autoxidation of 1,2,3-benzenetriol (pyrogallol) to produce oxygen radicals. These results were also reported in a later publication by Liang *et al.* (2000).[103]

4.21. Enzyme: hydrogenase (EC 1.18.99.1)

methyl viologen(red)(aq)=methyl viologen(ox)(aq) +H$_2$(g)

T/K	pH	K'
298.15	7.0	10
298.15	8.0	0.12
298.15	9.0	0.0013
298.15	9.85	$2.2\cdot10^{-5}$

Reference: Erbes and Burris (1978)[42]
Method: spectrophotometric and manometry
Buffer: Bes, Tricine, serine, glycine, and Mes
pH: 7.0–9.85
Evaluation: C

The values of K' given here are based on kinetic data

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(Haldane relation). The K' values given here were taken from Erbes and Burris' Fig. 7. Note that the standard state for this equilibrium constant uses atmospheres.

4.22. Enzyme: aspartate carbamoyl-transferase (EC 2.1.3.2)

carbamoyl phosphate(aq) + **L**-aspartate(aq) = orthophosphate(aq) + *N*-carbamoyl-**L**-aspartate(aq)

T/K	pH	K'
303.15	7.00	5900

Reference: Hsuanyu and Wedler (1987)[59]
Method: radioactivity
Buffer: Pipes (0.10 mol dm^{-3})
pH: 7.00
Evaluation: A

4.23. Enzyme: UDP-*N*-acetylglucosamine acyltransferase (EC 2.3.1.129)

(*R*)-3-hydroxytetradecanoyl-[acyl-carrier-protein](aq) + UDP-*N*-acetyl-**D**-glucosamine(aq) = acyl-carrier-protein(aq) + UDP-3-*O*-(3-hydroxytetradecanoyl)-*N*-acetyl-**D**-glucosamine(aq)

T/K	pH	K'
296.15	7.4	0.007
296.15	8.0	0.0095
296.15	8.5	0.004
296.15	9.0	0.002

Reference: Anderson *et al.* (1993)[71]
Method: radioactivity
Buffer: Hepes (0.10 mol dm^{-3}) or (Tris + HCl)
pH: 7.4
Evaluation: B

The values given here (see Table III of Anderson *et al.*) were obtained from measurement of K' from the forward reaction direction. Measurements from the reverse reaction direction gave values ranging from $K'=0.009$ to $K'=0.066$ at $T=296.15$ K and pH=7.40. The discrepancy in the forward and reverse equilibrium data may be due to thermal instability of UDP-3-*O*-(3-hydroxytetradecanoyl)-*N*-acetyl-**D**-glucosamine which has a half-life of 28 h at $T=303.15$ K and pH=6.0.

4.24. Enzyme: CO-methylating acetyl-CoA synthase (EC 2.3.1.169)

acetyl-CoA(aq) + corrinoid protein(aq) = carbon monoxide(aq) + methylcorrinoid protein(aq) + CoA(aq)

T/K	pH	K'_c
298.15	8.0	$2\cdot10^7$

Reference: Tan *et al.* (2006)[142]
Method: chromatography
Buffer: Tris (0.050*M*)
pH: 8.0
Evaluation: C

The value of K' is very approximate.

4.25. Enzyme: purine-nucleoside phosphorylase (EC 2.4.2.1)

2′-deoxyinosine(aq) + orthophosphate(aq) = hypoxanthine(aq) + 2-deoxy-α-**D**-ribose 1-phosphate(aq)

T/K	pH	K'
297.15	7.4	0.019

Reference: Friedkin (1950)[31]
Method: spectrophotometry
Buffer: Tris (0.030 mol dm^{-3}) + HCl
pH: 7.4
Evaluation: B

inosine(aq) + orthophosphate(aq) = hypoxanthine(aq) + α-**D**-ribose 1-phosphate(aq)

T/K	pH	K'
303.15	7.5	0.019

Reference: Kalckar (1947)[30]
Method: spectrophotometry
pH: 7.5
Evaluation: B

The value of K' given here is based on the results shown in Kalckar's Fig. 3.

4.26. Enzyme: uridine phosphorylase (EC 2.4.2.3)

uridine(aq) + orthophosphate(aq) = uracil(aq) + α-**D**-ribose 1-phosphate(aq)

T/K	pH	K'
303.15	7.56	0.58

Reference: Vita *et al.* (1983)[50]
Method: spectrophotometry
Buffer: Hepes (0.050 mol dm^{-3})
pH: 7.56
Evaluation: B

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The value of K' was obtained by using the Haldane relation.

4.27. Enzyme: adenine phosphoribosyltransferase (EC 2.4.2.7)

AMP(aq) + pyrophosphate(aq) = adenine(aq) + 5-phospho-α-**D**-ribose 1-diphosphate(aq)

T/K	pH	K'
303.15	7.4	0.0035

Reference: Hori and Henderson (1966)[34]
Method: radioactivity
Buffer: Tris (0.20 mol dm^{-3}) + HCl
pH: 7.4
Cofactor(s): $MgSO_4$ (0.0010 mol dm^{-3})
Evaluation: C

4.28. Enzyme: hypoxanthine phosphoribosyltransferase (EC 2.4.2.8)

IMP(aq) + pyrophosphate(aq) = hypoxanthine(aq) + 5-phospho-α-**D**-ribose 1-diphosphate(aq)

T/K	pH	K'
303.15	7.4	$3.3 \cdot 10^{-6}$

Reference: Xu *et al.* (1997)[78]
Method: radioactivity
Buffer: Tris (0.10 mol dm^{-3}) + HCl
pH: 7.4
Cofactor(s): $MgCl_2$ (0.012 mol dm^{-3})
Evaluation: B

The value of K' given here is approximate. The value $K' \approx 1.6 \cdot 10^5$ at T = 303.15 K and pH = 7.4 was also obtained by using the Haldane relation.

4.29. Enzyme: orotate phosphoribosyltransferase (EC 2.4.2.10)

orotidine 5′-phosphate(aq) + pyrophosphate(aq) = orotate(aq) + 5-phospho-α-**D**-ribose 1-diphosphate(aq)

T/K	pH	K'
303.15	8.0	9.3

Reference: Bhatia *et al.* (1990)[65]
Method: radioactivity
Buffer: Tris (0.075 mol dm^{-3}) + HCl
pH: 8.0
Cofactor(s): $MgCl_2$ (0.0060 mol dm^{-3})
Evaluation: B

4.30. Enzyme: nicotinate phosphoribosyltransferase (EC 2.4.2.11)

β-nicotinamide mononucleotide(aq) + pyrophosphate(aq) = nicotinic acid(aq) + 5-phospho-α-**D**-ribose 1-diphosphate(aq)

T/K	pH	K'
303.15	8.0	1.5

Reference: Vinitsky and Grubmeyer (1993)[72]
Method: radioactivity
Buffer: Tris
pH: 8.0
Cofactor(s): Mg^{2+}
Evaluation: C

4.31. Enzyme: 5′-methylthioadenosine phosphorylase (EC 2.4.2.28)

5′-methylthioadenosine(aq) + orthophosphate(aq) = adenine(aq) + 5-methylthio-**D**-ribose 1-phosphate(aq)

T/K	pH	K'
310.15	7.4	0.0139

Reference: Ragione *et al.* (1986)[57]
Method: chromatography and radioactivity
Buffer: Tris (0.050 mol dm^{-3}) + HCl
pH: 7.4
Evaluation: B

4.32. Enzyme: 4-aminobutyrate transaminase (EC 2.6.1.19)

4-aminobutanoate(aq) + 2-oxoglutarate(aq) = 4-oxobutanoate(aq) + **L**-glutamate(aq)

T/K	pH	K'
298.15	8.5	0.29

Reference: 72DUF/NEL
Method: enzymatic assay
Buffer: glycylglycine (0.12 mol dm^{-3})
pH: 8.6
Evaluation: B

4-aminobutanoate(aq) + 2-oxoglutarate(aq) = 4-oxobutanoate(aq) + **L**-glutamate(aq)

T/K	pH	K'
295.15	8.5	0.04

Reference: Van der Laan *et al.* (1979)[45]
Method: spectrophotometry and radioactivity
Buffer: Tris (0.050 mol dm^{-3}) + HCl

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pH: 8.5
Evaluation: B

This result is based on kinetic data (Haldane relation).

4-aminobutanoate(aq)+2-oxoglutarate(aq)
=4-oxobutanoate(aq)+L-glutamate(aq)

T/K	pH	K'
295.15	8.5	0.04

Reference: van Bemmelen *et al.* (1985)[56]
Method: chromatography and spectrophotometry
Buffer: Tris (0.050 mol dm^{-3})+HCl
pH: 8.5
Evaluation: C

The apparent equilibrium constant was obtained by using the Haldane relation.

4.33. Enzyme: (2-aminoethyl)phosphonate-pyruvate transferase (EC 2.6.1.37)

(2-aminoethyl)phosphonate(aq)+pyruvate(aq)
=2-phosphonoacetaldehyde(aq)+L-alanine(aq)

T/K	pH	K'
298.15	8.5	0.5

Reference: Kim *et al.* (2002)[114]
Method: spectrophotometry
Buffer: Tricine (0.050 mol dm^{-3})
pH: 8.5
Cofactor(s): $MgCl_2$ (0.0050 mol dm^{-3})
Evaluation: B

This approximate result is based on kinetic data (Haldane relation).

4.34. Enzyme: branched-chain-amino-acid transferase (EC 2.6.1.42)

L-leucine(aq)+2-oxoglutarate(aq)=2-oxoisocaproate(aq)
+L-glutamate(aq)

T/K	pH	I_m/(mol kg^{-1})	K'
298.15	7.19	0.31	2.42

Reference: Tewari *et al.* (2000)[108]
Method: calorimetry and chromatography
Buffer: phosphate
pH: 7.21
Cofactor(s): pyridoxal 5-phosphate
Evaluation: A

Tewari *et al.* also calculated K=4.85, $\Delta_r G^\circ$=−3.91 kJ mol^{-1}, $\Delta_r H^\circ$=6.0 kJ mol^{-1}, and $\Delta_r S^\circ$=33.2 J K^{-1} mol^{-1} for the chemical reference reaction [L-leucine$^{\pm}$(aq)+2-oxoglutarate^{2-}(aq)
=2-oxoisocaproate^{-}(aq)+L-glutamate^{-}(aq)] at T=298.15 K and I=0.

L-leucine(aq)+2-oxoglutarate(aq)=2-oxoisocaproate(aq)
+L-glutamate(aq)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.20	0.31	5.12

Reference: Tewari *et al.* (2000)[108]
Method: calorimetry and chromatography
Buffer: phosphate
pH: 7.21
Cofactor(s): pyridoxal 5-phosphate
Evaluation: A

Tewari *et al.* also calculated K=4.85, $\Delta_r G^\circ$=−3.91 kJ mol^{-1}, $\Delta_r H^\circ$=6.0 kJ mol^{-1}, and $\Delta_r S^\circ$=33.2 J K^{-1} mol^{-1} for the chemical reference reaction [L-leucine$^{\pm}$(aq)+2-oxoglutarate^{2-}(aq)
=2-oxoisocaproate^{-}(aq)+L-glutamate^{-}(aq)] at T=298.15 K and I=0.

L-*tert*-leucine(aq)+2-oxoglutarate(aq)
=3,3-dimethyl-2-oxobutanoate(aq)+L-glutamate(aq)

T/K	pH	I_m/(mol kg^{-1})	K'
298.15	7.19	0.31	6.01

Reference: Tewari *et al.* (2000)[108]
Method: calorimetry and chromatography
Buffer: phosphate
pH: 7.21
Cofactor(s): pyridoxal 5-phosphate
Evaluation: A

Tewari *et al.* also calculated K=12.1, $\Delta_r G^\circ$=−6.18 kJ mol^{-1}, $\Delta_r H^\circ$=4.9 kJ mol^{-1}, and $\Delta_r S^\circ$=37.2 J K^{-1} mol^{-1} for the chemical reference reaction [L-*tert*-leucine$^{\pm}$(aq)+2-oxoglutarate^{2-}(aq)
=3,3-dimethyl-2-oxobutanoate^{-}(aq)+L-glutamate^{-}(aq)] at T=298.15 K and I=0.

L-*tert*-leucine(aq)+2-oxoglutarate(aq)
=3,3-dimethyl-2-oxobutanoate(aq)+L-glutamate(aq)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.20	0.31	4.00

Reference: Tewari *et al.* (2000)[108]
Method: calorimetry and chromatography

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Buffer: phosphate
pH: 7.21
Cofactor(s): pyridoxal 5-phosphate
Evaluation: A

Tewari *et al.* also calculated $K=12.1$, $\Delta_r G^\circ = -6.18$ kJ mol^{-1}, $\Delta_r H^\circ = 4.9$ kJ mol^{-1}, and $\Delta_r S^\circ = 37.2$ J K^{-1} mol^{-1} for the chemical reference reaction [**L**-*tert*-leucine$^{\pm}$(aq)+2-oxoglutarate^{2-}(aq) =3,3-dimethyl-2-oxobutanoate^{-}(aq)+**L**-glutamate^{-}(aq)] at $T=298.15$ K and $I=0$.

L-valine(aq)+2-oxoglutarate(aq)=2-oxovalerate(aq) +**L**-glutamate(aq)

T/K	pH	I_m/(mol kg^{-1})	K'
298.15	7.21	0.31	1.67

Reference: Tewari *et al.* (2000)[108]
Method: calorimetry and chromatography
Buffer: phosphate
pH: 7.21
Cofactor(s): pyridoxal 5-phosphate
Evaluation: A

Tewari *et al.* also calculated $K=3.33$, $\Delta_r G^\circ = -2.98$ kJ mol^{-1}, $\Delta_r H^\circ = 5.7$ kJ mol^{-1}, and $\Delta_r S^\circ = 29.1$ J K^{-1} mol^{-1} for the chemical reference reaction [**L**-valine$^{\pm}$(aq)+2-oxoglutarate^{2-}(aq)=2-oxoisovalerate^{-}(aq) +**L**-glutamate^{-}(aq)] at $T=298.15$ K and $I=0$.

L-valine(aq)+2-oxoglutarate(aq)=2-oxovalerate(aq) +**L**-glutamate(aq)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_r H$(cal)/(kg mol^{-1})
298.15	7.21	0.31	4.84

Reference: Tewari *et al.* (2000)[108]
Method: calorimetry and chromatography
Buffer: phosphate
pH: 7.21
Cofactor(s): pyridoxal 5-phosphate
Evaluation: A

Tewari *et al.* also calculated $K=3.33$, $\Delta_r G^\circ = -2.98$ kJ mol^{-1}, $\Delta_r H^\circ = 5.7$ kJ mol^{-1}, and $\Delta_r S^\circ = 29.1$ J K^{-1} mol^{-1} for the chemical reference reaction [**L**-valine$^{\pm}$(aq)+2-oxoglutarate^{2-}(aq)=2-oxoisovalerate^{-}(aq) +**L**-glutamate^{-}(aq)] at $T=298.15$ K and $I=0$.

4.35. Enzyme: phosphoserine transferase (EC 2.6.1.52)

O-phospho-**L**-serine(aq)+2-oxoglutarate(aq) =3-phosphono-oxypyruvate(aq)+**L**-glutamate(aq)

T/K	pH	K'
305	7.8	0.025

Reference: Basurko *et al.* (1999)[86]
Method: spectrophotometry
Buffer: (Tris+HCl) and (Hepes+KOH)
pH: 7.5–8.1
Evaluation: C

This result is based on kinetic data (Haldane relation). The kinetic measurements were performed at temperatures ranging from $T=298.15$ K to $T=311.15$ K and at pH=7.5 and pH=8.1. However, the actual temperature and pH to which the measured value of K' refers were not specified. We have assumed that the value of K' refers to the respective averages of the aforementioned temperatures and pHs.

4.36. Enzyme: glucokinase (EC 2.7.1.2)

ATP(aq)+**D**-glucose(aq)=ADP(aq) +**D**-glucose 6-phosphate(aq)

T/K	pH	Buffer	Enzyme	c(KCl)/(mol dm^{-3})	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.6	phosphate	Hxk1	0	−25.0
298.15	7.6	phosphate	Hxk2	0	−19.9
298.15	7.6	Hepes	Hxk1	0	−40.8
298.15	7.6	Hepes	Hxk2	0	−32.4
298.15	7.6	Mops	Hxk1	0	−42.9
298.15	7.6	Mops	Hxk2	0	−33.4
298.15	7.6	imidazole	Hxk1	0	−54.4
298.15	7.6	imidazole	Hxk2	0	−47.0
298.15	7.6	Tris	Hxk1	0	−65.9
298.15	7.6	Tris	Hxk2	0	−49.2
298.15	7.6	Tris	Hxk1	0	−61.15
298.15	7.6	Mops	Hxk2	0	−33.79
298.15	7.6	Tris	Hxk1	0.025	−62.76
298.15	7.6	Mops	Hxk2	0.025	−32.18
298.15	7.6	Tris	Hxk1	0.050	−67.91
298.15	7.6	Mops	Hxk2	0.050	−32.18
298.15	7.6	Tris	Hxk1	0.075	−61.15
298.15	7.6	Mops	Hxk2	0.075	−33.79
298.15	7.6	Tris	Hxk1	0.100	−63.56
298.15	7.6	Mops	Hxk2	0.100	−32.99
298.15	7.6	Tris	Hxk1	0.125	−66.46
298.15	7.6	Mops	Hxk2	0.125	−32.18
298.15	7.6	Tris	Hxk1	0.150	−67.59
298.15	7.6	Mops	Hxk2	0.150	−33.79
298.15	7.6	Tris	Hxk1	0.175	−63.56
298.15	7.6	Mops	Hxk2	0.175	−33.79
298.15	7.6	Tris	Hxk1	0.200	−67.59
298.15	7.6	Mops	Hxk2	0.200	−32.99

Reference: Bianconi (2003)[119]
Method: calorimetry
Buffer: Hepes, imidazole, Mops, phosphate, and Tris
pH: 7.6

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Cofactor(s): $MgCl_2$ (0.005 mol dm^{-3})
Evaluation: B

The values of $\Delta_r H$(cal) given here were read from Bianconi's Figs. 2 and 5. Two different isozymes of glucokinase (Hxk1 and Hxk2) were used. Interestingly, the results differed. Since a true catalyst cannot change the position of equilibrium or the standard molar enthalpy of reaction, some experimental factor must have caused the differences in the values of $\Delta_r H$(cal).

4.37. Enzyme: protein kinase (EC 2.7.1.37)

ATP(aq) + serpeptide(aq) = ADP(aq) + phosphorylated serpeptide(aq)

T/K	pH	K'
298.15	6.0	160
298.15	7.2	2400

Reference: Qamar *et al.* (1992)[69]
Method: spectrophotometry; NMR
Buffer: Mes (0.10 mol dm^{-3})
pH: 6.0–7.0
Cofactor(s): $MgCl_2$
Evaluation: A

Serpeptide is Leu-Arg-Arg-Ala-Ser-Leu-Gly. The values of K' given here are the respective averages of the values obtained by using two different methods as well as the Haldane relation.

ATP(aq) + syntide 2(aq) = ADP(aq) + phosphosyntide(aq)

T/K	pH	K'
298.15	7.5	3500

Reference: Kwiatkowski *et al.* (1990)[66]
Method: radioactivity
Buffer: Hepes (0.05 mol dm^{-3})
pH: 7.5
Cofactor(s): $MgCl_2$
Evaluation: C

Syntide 2 is Pro-Leu-Ala-Arg-Thr-Leu-Ser-Val-Ala-Gly-Leu-Pro-Gly-Lys-Lys. This approximate value of K' is based on kinetic data (Haldane relation).

4.38. Enzyme: pyruvate kinase (EC 2.7.1.40)

ATP(aq) + pyruvate(aq) = phospho*enol*pyruvate(aq) + ADP(aq)

T/K	pH	pMg	I_c/(mol dm^{-3})	K'
298.15	6.98	3.22	···	$3.01 \cdot 10^{-5}$
298.15	6.94	3.26	···	$2.82 \cdot 10^{-5}$
278.43	7.00	3.0	0.25	$2.25 \cdot 10^{-5}$
280.13	7.00	3.0	0.25	$2.46 \cdot 10^{-5}$
298.15	7.00	3.0	0.25	$2.65 \cdot 10^{-5}$
307.93	7.00	3.0	0.25	$2.74 \cdot 10^{-5}$
318.14	7.00	3.0	0.25	$2.84 \cdot 10^{-5}$
298.15	6.40	3.0	0.25	$1.11 \cdot 10^{-4}$
298.15	6.70	3.0	0.25	$6.98 \cdot 10^{-5}$
298.15	7.00	3.0	0.25	$2.78 \cdot 10^{-5}$
298.15	7.40	3.0	0.25	$1.58 \cdot 10^{-5}$
298.15	7.80	3.0	0.25	$1.03 \cdot 10^{-5}$

Reference: Dobson *et al.* (2002)[112]
Method: spectrophotometry and enzymatic assay
Buffer: phosphate
pH: 6.40–7.80
Cofactor(s): $MgCl_2$
Evaluation: A

Except for the first two values, the K' values given here were obtained from Figs. 1 and 2 of Dobson *et al.* Dobson *et al.* also calculated $K = 9.17 \cdot 10^{-12}$, $\Delta_r G^\circ = 63.0$ kJ mol^{-1}, $\Delta_r H^\circ = 6.43$ kJ mol^{-1}, and $\Delta_r S^\circ = -190$ J K^{-1} mol^{-1} at $T = 298.15$ K and $I = 0$ for the chemical reference reaction [ATP^{4-}(aq) + pyruvate$^-$(aq) = phospho*enol*pyruvate^{3-}(aq) + ADP^{3-}(aq) + H^+].

4.39. Enzyme: pyrophosphate-fructose-6-phosphate 1-phosphotransferase (EC 2.7.1.90)

pyrophosphate(aq) + **D**-fructose 6-phosphate(aq) = orthophosphate(aq) + **D**-fructose 1,6-bisphosphate(aq)

T/K	pH	K'
298.15	8.0	0.006

Reference: Bertagnolli and Cook (1984)[51]
Method: spectrophotometry and NMR
Buffer: Taps
pH: 8.0
Cofactor(s): $MgCl_2$
Evaluation: B

The apparent equilibrium constant was measured both by using NMR and by using the Haldane relation. The values obtained by using these respective methods were $K' = 0.007$ and $K' = 0.005$. The average of these two results is given here.

4.40. Enzyme: myosin-light-chain kinase (EC 2.7.1.117)

ATP(aq) + myosin light chain(aq) = ADP(aq) + myosin light chain phosphate(aq)

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T/K	pH	K'
303.15	7.2	59

Reference: Geuss *et al.* (1985)[54]
Method: radioactivity
Buffer: Hepes+KOH
pH: 7.2
Cofactor(s): Ca^{2+} and calmodulin
Evaluation: B

Geuss *et al.* also obtained the value $K' \approx 70$ by using the Haldane relation.

4.41. Enzyme: actinomycin synthetase I (EC 2.7.2.a)

2-aminobenzoic acid(aq)+ATP(aq)
=2-aminobenzoic acid adenylate(aq)+pyrophosphate(aq)

T/K	pH	K'
301.15	6.8	$1.5 \cdot 10^{-5}$

Reference: Keller and Schlumbohm (1992)[68]
Method: radioactivity
Buffer: potassium phosphate (0.050 mol dm^{-3})
pH: 6.8
Cofactor(s): $MgCl_2$ (0.010 mol dm^{-3})
Evaluation: B

3-aminobenzoic acid(aq)+ATP(aq)
=3-aminobenzoic acid adenylate(aq)+pyrophosphate(aq)

T/K	pH	K'
301.15	6.8	$1 \cdot 10^{-6}$

Reference: Keller and Schlumbohm (1992)[68]
Method: radioactivity
Buffer: potassium phosphate (0.050 mol dm^{-3})
pH: 6.8
Cofactor(s): $MgCl_2$ (0.010 mol dm^{-3})
Evaluation: B

4-aminobenzoic acid(aq)+ATP(aq)
=4-aminobenzoic acid adenylate(aq)+pyrophosphate(aq)

T/K	pH	K'
301.15	6.8	$1.0 \cdot 10^{-3}$

Reference: Keller and Schlumbohm (1992)[68]
Method: radioactivity
Buffer: potassium phosphate (0.050 mol dm^{-3})
pH: 6.8
Cofactor(s): $MgCl_2$ (0.010 mol dm^{-3})
Evaluation: B

benzoic acid(aq)+ATP(aq)=benzoic acid adenylate(aq)
+pyrophosphate(aq)

T/K	pH	K'
301.15	6.8	$1 \cdot 10^{-5}$

Reference: Keller and Schlumbohm (1992)[68]
Method: radioactivity
Buffer: potassium phosphate (0.050 mol dm^{-3})
pH: 6.8
Cofactor(s): $MgCl_2$ (0.010 mol dm^{-3})
Evaluation: B

2,3-dihydroxybenzoic acid(aq)+ATP(aq)
=2,3-dihydroxybenzoic acid adenylate(aq)
+pyrophosphate(aq)

T/K	pH	K'
301.15	6.8	$4 \cdot 10^{-6}$

Reference: Keller and Schlumbohm (1992)[68]
Method: radioactivity
Buffer: potassium phosphate (0.050 mol dm^{-3})
pH: 6.8
Cofactor(s): $MgCl_2$ (0.010 mol dm^{-3})
Evaluation: B

3-hydroxyanthranilic acid(aq)+ATP(aq)
=3-hydroxyanthranilic acid adenylate(aq)
+pyrophosphate(aq)

T/K	pH	K'
301.15	6.8	$5.8 \cdot 10^{-4}$

Reference: Keller and Schlumbohm (1992)[68]
Method: radioactivity
Buffer: potassium phosphate (0.050 mol dm^{-3})
pH: 6.8
Cofactor(s): $MgCl_2$ (0.010 mol dm^{-3})
Evaluation: B

3-hydroxybenzoic acid(aq)+ATP(aq)=3-hydroxybenzoic acid adenylate(aq)+pyrophosphate(aq)

T/K	pH	K'
301.15	6.8	$1.7 \cdot 10^{-4}$

Reference: Keller and Schlumbohm (1992)[68]

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Method: radioactivity
Buffer: potassium phosphate (0.050 mol dm^{-3})
pH: 6.8
Cofactor(s): $MgCl_2$ (0.010 mol dm^{-3})
Evaluation: B

4-hydroxybenzoic acid(aq)+ATP(aq)=4-hydroxybenzoic acid adenylate(aq)+pyrophosphate(aq)

T/K	pH	K'
301.15	6.8	$4.1 \cdot 10^{-4}$

Reference: Keller and Schlumbohm (1992)[68]
Method: radioactivity
Buffer: potassium phosphate (0.050 mol dm^{-3})
pH: 6.8
Cofactor(s): $MgCl_2$ (0.010 mol dm^{-3})
Evaluation: B

3-hydroxy-4-methylbenzoic acid(aq)+ATP(aq) =3-hydroxy-4-methylbenzoic acid adenylate(aq)+pyrophosphate(aq)

T/K	pH	K'
277.0	6.8	0.004 60
284.7	6.8	0.004 59
293.0	6.8	0.003 81
301.2	6.8	0.003 19

Reference: Keller and Schlumbohm (1992)[68]
Method: radioactivity
Buffer: potassium phosphate (0.050 mol dm^{-3})
pH: 6.8
Cofactor(s): $MgCl_2$ (0.010 mol dm^{-3})
Evaluation: B

The values of K' given here were read from Keller and Schlumbohm's Fig. 5. Keller and Schlumbohm also calculated $\Delta_r H'^\circ = -15.5$ kJ mol^{-1} from the temperature dependence of K'.

3-methylbenzoic acid(aq)+ATP(aq)=3-methylbenzoic acid adenylate(aq)+pyrophosphate(aq)

T/K	pH	K'
301.15	6.8	$2.1 \cdot 10^{-4}$

Reference: Keller and Schlumbohm (1992)[68]
Method: radioactivity
Buffer: potassium phosphate (0.050 mol dm^{-3})
pH: 6.8
Cofactor(s): $MgCl_2$ (0.010 mol dm^{-3})
Evaluation: B

4-methylbenzoic acid(aq)+ATP(aq)=4-methylbenzoic acid adenylate(aq)+pyrophosphate(aq)

T/K	pH	K'
301.15	6.8	$5.4 \cdot 10^{-4}$

Reference: Keller and Schlumbohm (1992)[68]
Method: radioactivity
Buffer: potassium phosphate (0.050 mol dm^{-3})
pH: 6.8
Cofactor(s): $MgCl_2$ (0.010 mol dm^{-3})
Evaluation: B

4.42. Enzyme: creatine kinase (EC 2.7.3.2)

ATP(aq)+creatine(aq)=ADP(aq)+phosphocreatine(aq)

T/K	pH	K'
298.15	9.0	0.335

Reference: Liang *et al.* (2000)[102]
Method: calorimetry
Buffer: glycine+NaOH
pH: 9.0
Cofactor(s): $MgCl_2$
Evaluation: C

ATP(aq)+creatine(aq)=ADP(aq)+phosphocreatine(aq))

T/K	pH	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	9.0	−24.8

Reference: Liang *et al.* (2000)[102]
Method: calorimetry
Buffer: glycine+NaOH
pH: 9.0
Cofactor(s): $MgCl_2$
Evaluation: B

4.43. Enzyme: arginine kinase (EC 2.7.3.3)

ATP(aq)+**L**-arginine(aq)=ADP(aq) +N^ω-phospho-**L**-arginine(aq)

T/K	pH	$\frac{c(Mg^{2+})}{(\text{mol dm}^{-3})}$	$\frac{I_c}{(\text{mol dm}^{-3})}$	K'
298.15	7.13	0.005 65	0.25	0.0277
278.15	7.00	0.001 0	0.25	0.0221
288.15	7.00	0.001 0	0.25	0.0252
298.15	7.00	0.001 0	0.25	0.0282
306.15	7.00	0.001 0	0.25	0.0299
313.15	7.00	0.001 0	0.25	0.0334

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T/K	pH	$\frac{c(Mg^{2+})}{(mol\ dm^{-3})}$	$\frac{I_c}{(mol\ dm^{-3})}$	K'
298.15	6.4	0.001 0	0.25	0.0103
298.15	6.7	0.001 0	0.25	0.0173
298.15	7.0	0.001 0	0.25	0.0321
298.15	7.4	0.001 0	0.25	0.0725
298.15	7.8	0.001 0	0.25	0.174
298.15	8.2	0.001 0	0.25	0.465
298.15	7.0	0.000 10	0.25	0.0903
298.15	7.0	0.000 25	0.25	0.0606
298.15	7.0	0.000 50	0.25	0.0445
298.15	7.0	0.001 0	0.25	0.0307
298.15	7.0	0.002 0	0.25	0.0252
298.15	7.0	0.004 0	0.25	0.0215

Reference: Teague and Dobson (1999)[95]
Method: spectrophotometry
Buffer: potassium phosphate (0.050 mol dm^{-3})
pH: 6.4–8.2
Cofactor(s): $MgCl_2$
Evaluation: A

Teague and Dobson also calculated $\Delta_r G^\circ = 45.01$ kJ mol^{-1}, $\Delta_r H^\circ = 16.10$ kJ mol^{-1}, and $\Delta_r S^\circ = -97.6$ J K^{-1} mol^{-1} for the chemical reference reaction [$ATP^{4-}(aq) + $ **L**-arginine(aq) = $ADP^{3-}(aq) + N^\omega$-phospho-**L**-$arginine^{2-}(aq) + H^+(aq)$] at $T = 298.15$ K and $I = 0.25$ mol dm^{-3}.

4.44. Enzyme: sulfate adenylyltransferase (EC 2.7.7.4)

ATP(aq) + sulfate(aq) = pyrophosphate(aq) + adenylylsulfate(aq)

T/K	pH	K'
303.15	8.0	$2.5 \cdot 10^{-9}$

Reference: Farley *et al.* (1976)[40]
Method: radioactivity
Buffer: Tris + HCl
pH: 8.0
Cofactor(s): Mg^{2+}
Evaluation: B

Farley *et al.* also used the Haldane relation to obtain $K' \approx 2 \cdot 10^{-8}$ at $T = 303.15$ K and pH = 8.0.

4.45. Enzyme: DNA-directed DNA polymerase (EC 2.7.7.7)

deoxynucleoside triphosphate(aq) + poly[d-(A-T)]n(aq) = pyrophosphate(aq) + poly[(d-(A-T))]n+1(aq)

T/K	pH	K'
310.15	7.5	500

Reference: McClure and Jovin (1975)[38]
Method: radioactivity
Buffer: potassium phosphate (0.075 mol dm^{-3})
pH: 7.5
Cofactor(s): $MgCl_2$ (0.0075 mol dm^{-3})
Evaluation: C

The substance poly[d-(A-T)] is an alternating purine-pyrimidine polydeoxyribonucleotide of adenine and thymine. The value of K' is based on the measured ratio [c(pyrophosphate)/c(deoxynucleoside triphosphate)]. Thus, the value of K' assumes that $c[\text{poly(d-A-T)}_{n+1}]/c[\text{poly(d-A-T)}_n] = 1$. McClure and Jovin also used kinetic data and the Haldane relation to obtain $K' \approx 2000$ under the conditions given here.

4.46. Enzyme: ADP-glucose phosphorylase (EC 2.7.7.a)

ADP(aq) + α-**D**-glucose 1-phosphate(aq) = ADPglucose(aq) + orthophosphate(aq)

T/K	pH	$c(MgCl_2)$/(mol dm^{-3})	K'
298.15	7.0	0	0.2
298.15	7.0	0.0001	0.025

Reference: McCoy *et al.* (2006)[138]
Method: spectrophotometry and enzymatic assay
Buffer: Hepes (0.1 mol dm^{-3})
pH: 7.0
Cofactor(s): $MgCl_2$
Evaluation: B

4.47. Enzyme: pyruvate, water dikinase (EC 2.7.9.2)

ATP(aq) + pyruvate(aq) + H_2O(l) = AMP(aq) + phospho*enol*pyruvate(aq) + orthophosphate(aq)

T/K	pH	K'_c
323.15	6.5	52

Reference: Sakuraba *et al.* (1999)[94]
Method: enzymatic assay
Buffer: Bis-Tris (0.10 mol dm^{-3})
pH: 6.5
Evaluation: C

The value of K' given here was calculated from the concentrations of the reactants and products reported by Sakuraba *et al.* Note that they included the concentration of water in their calculation of K'_c.

4.48. Enzyme: triacylglycerol lipase (EC 3.1.1.3)

benzyl alcohol(sln) + butyl acetate(sln) = benzyl acetate(sln) + 1-butanol(sln)

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T/K	K
303.15	0.248
308.15	0.236
313.15	0.245
318.15	0.256

Reference: Tewari *et al.* (2004)[131]
Method: chromatography
Evaluation: A

This reaction was carried out in supercritical carbon dioxide (P=10.0 MPa). Tewari *et al.* also calculated $\Delta_r G^\circ$ =3.56 kJ mol^{-1}, $\Delta_r H^\circ$=2.1 kJ mol^{-1}, and $\Delta_r S^\circ$= −4.9 J K^{-1} mol^{-1} at T=298.15 K for this reaction.

benzyl alcohol(sln)+butyl acetate(sln)=benzyl acetate(sln)+1-butanol(sln)

T/K	Solvent	K
292.95	*n*-hexane	0.317
298.15	*n*-hexane	0.310
303.15	*n*-hexane	0.317
308.15	*n*-hexane	0.319
298.15	neat reaction mixture	0.294
298.15	carbon tetrachloride	0.305
298.15	acetonitrile	0.299
298.15	*tert*-butyl methyl ether	0.237
298.15	2-butanone	0.281

Reference: Tewari *et al.* (2003)[126]
Method: chromatography
Evaluation: A

Here "sln" refers to the several organic solvents used in this study. Tewari *et al.* calculated $\Delta_r G^\circ$=2.86 kJ mol^{-1}, $\Delta_r H^\circ$=0.6 kJ mol^{-1}, and $\Delta_r S^\circ$=−7.6 J K^{-1} mol^{-1} for this reaction carried out in *n*-hexane at T=298.15 K.

butyl decanoate(sln)+H_2O(sln)=1-butanol(sln)+1-decanoic acid(sln)

T/K	Solvent	K
323.15	2-methyl-2-butanol	0.518
323.15	2-methylpropan-2-ol	0.714
323.15	butyronitrile	0.0265
323.15	propionitrile	0.0469
323.15	acetonitrile	0.0446
323.15	1,4-dioxane	0.269
323.15	2-methylpropan-2-ol (x=0.795)+acetonitrile (x=0.205)	0.435
323.15	2-methylpropan-2-ol (x=0.624)+acetonitrile (x=0.376)	0.356
323.15	2-methylpropan-2-ol (x=0.357)+acetonitrile (x=0.643)	0.230
323.15	2-methylpropan-2-ol (x=0.156)+acetonitrile (x=0.844)	0.125
323.15	2-methylpropan-2-ol (x=0.624)+propionitrile (x=0.376)	0.463
323.15	2-methylpropan-2-ol (x=0.156)+propionitrile (x=0.844)	0.144
323.15	2-methylpropan-2-ol (x=0.624)+butyronitrile (x=0.376)	0.377
323.15	2-methylpropan-2-ol (x=0.156)+butyronitrile (x=0.844)	0.159
323.15	2-methyl-2-butanol (x=0.526)+acetonitrile (x=0.474)	0.289
323.15	2-methyl-2-butanol (x=0.156)+acetonitrile (x=0.844)	0.122
323.15	2-methyl-2-butanol (x=0.846)+butyronitrile (x=0.154)	0.400
323.15	2-methyl-2-butanol (x=0.101)+butyronitrile (x=0.899)	0.0952

Reference: Kobayashi *et al.* (2003)[122]
Method: spectrophotometry and Karl Fischer
Evaluation: A

The values of K given here are shown in Figs. 3 and 4 of Kobayashi *et al.*[122] The quantity x is the mole fraction of a given substance in the solvent. The numerical values are from a private communication from Adachi (2006).[135]

1,2-dioctanoyl glycerol(sln)+2 H_2O(sln)=glycerol(sln)+2 *n*-octanoic acid(sln)

T/K	Solvent	K
310.15	acetonitrile	0.0709
310.15	benzene	1.042
310.15	toluene	0.885
310.15	neat reaction mixture	0.676

Reference: Tewari and Bunk[109]
Method: chromatography
Evaluation: A

1,2-dioctanoyl glycerol(sln)+H_2O(sln)=1-mono-octanoyl glycerol(sln)+*n*-octanoic acid(sln)

T/K	Solvent	K
310.15	acetonitrile	0.286
310.15	benzene	0.408
310.15	toluene	0.397
310.15	neat reaction mixture	1.02

Reference: Tewari and Bunk[109]
Method: chromatography
Evaluation: A

1,2-dioctanoyl glycerol(sln)+H_2O(sln)=2-mono-octanoyl glycerol(sln)+*n*-octanoic acid(sln)

T/K	Solvent	K
310.15	acetonitrile	0.15
310.15	benzene	0.20
310.15	toluene	0.20
310.15	neat reaction mixture	0.51

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Reference: Tewari and Bunk[109]
Method: chromatography
Evaluation: A

1,3-dioctanoyl glycerol(sln) + 2 H_2O(sln) = glycerol(sln) + 2 *n*-octanoic acid(sln)

T/K	Solvent	*K*
310.15	acetonitrile	0.0483
310.15	benzene	0.714
310.15	toluene	0.602
310.15	neat reaction mixture	0.455

Reference: Tewari and Bunk[109]
Method: chromatography
Evaluation: A

1,3-dioctanoyl glycerol(sln) + H_2O(sln) = 1-mono-octanoyl glycerol(sln) + *n*-octanoic acid(sln)

T/K	Solvent	*K*
310.15	acetonitrile	0.20
310.15	benzene	0.28
310.15	toluene	0.27
310.15	neat reaction mixture	0.69

Reference: Tewari and Bunk[109]
Method: chromatography
Evaluation: A

dodecyl dodecanoate(sln) + H_2O(sln) = 1-dodecanol(sln) + 1-dodecanoic acid(sln)

T/K	Solvent	*K*
298.15	hexane	0.0253
298.15	heptane	0.0283
298.15	cyclohexane	0.0429
298.15	2,2,4-trimethylpentane	0.0368
298.15	toluene	0.0559

Reference: Tewari (1998)[84]
Method: chromatography
Evaluation: A

D-glucose(sln) + 1-dodecanoic acid(sln) = 1-dodecanoyl D-glucose ester(sln) + H_2O(sln)

T/K	*K*
333.15	0.30

Reference: Flores and Halling (2002)[113]
Method: gas chromatography and Karl Fischer
Evaluation: A

Here "sln" is 2-methl 2-butanol.

(−)-menthol(sln) + 1-dodecanoic acid(sln) = (−)-menthyl dodecanoate(sln) + H_2O(sln)

T/K	Solvent	*K*
298.15	hexane	6.5
298.15	heptane	21.7
298.15	cyclohexane	23.7
298.15	2,2,4-trimethylpentane	16.2
298.15	toluene	12.0
298.15	acetonitrile	3.23
298.15	2-methyl-2-butanol	5.82

Reference: Tewari *et al.* (1999)[96]
Method: chromatography
Evaluation: A

Here "sln" refers to the several organic solvents used in this study.

(−)-menthol(sln) + dodecyl dodecanoate(sln) = (−)-menthyl dodecanoate(sln) + 1-dodecanol(sln)

T/K	Solvent	*K*
287.85	2,2,4-trimethyl pentane	0.333
293.55	2,2,4-trimethyl pentane	0.368
298.05	2,2,4-trimethyl pentane	0.359
303.30	2,2,4-trimethyl pentane	0.345
298.15	*n*-hexane	0.362
282.95	*n*-heptane	0.378
288.15	*n*-heptane	0.387
293.15	*n*-heptane	0.407
298.15	*n*-heptane	0.410
282.95	toluene	0.359
288.15	toluene	0.365
293.15	toluene	0.356
298.15	toluene	0.364

Reference: Tewari (2000)[105]
Method: chromatography
Evaluation: A

Tewari also calculated $K=0.353$, $\Delta_r G^\circ = 2.58$ kJ mol^{-1}, $\Delta_r H^\circ = 1.5$ kJ mol^{-1}, and $\Delta_r S^\circ = -4$ J K^{-1} mol^{-1} for this reaction carried out in 2,2,4-trimethylpentane; $K=0.412$, $\Delta_r G^\circ = 2.20$ kJ mol^{-1}, $\Delta_r H^\circ = 4.0$ kJ mol^{-1}, and $\Delta_r S^\circ = 6$ J K^{-1} mol^{-1} for this reaction carried out in *n*-heptane; and $K=0.361$, $\Delta_r G^\circ = 2.53$ kJ mol^{-1}, $\Delta_r H^\circ = 0.2$ kJ mol^{-1}, and $\Delta_r S^\circ = -8$ J K^{-1} mol^{-1} for this reaction carried out in toluene. In all cases, $T=298.15$ K.

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1-mono-octanoyl glycerol(sln)+H_2O(sln)=glycerol(sln)+*n*-octanoic acid(sln)

T/K	Solvent	*K*
310.15	acetonitrile	0.257
310.15	benzene	2.50
310.15	toluene	2.17
310.15	neat reaction mixture	0.69

Reference: Tewari and Bunk[109]
Method: chromatography
Evaluation: A

2-mono-octanoyl glycerol(sln)+H_2O(sln)=glycerol(sln)+*n*-octanoic acid(sln)

T/K	Solvent	*K*
310.15	acetonitrile	0.515
310.15	benzene	5.00
310.15	toluene	4.35
310.15	neat reaction mixture	1.37

Reference: Tewari and Bunk[109]
Method: chromatography
Evaluation: A

oleic acid(sln)+1-butanol(sln)=1-butyl oleate(sln)+H_2O(sln)

T/K	*K*
308.15	91

Reference: Flores *et al.* (2000)[99]
Method: gas chromatography; Karl Fischer
Evaluation: B

Here "sln" is 1-butanol.

(*R*)-(+)-1-phenyl-1-butanol(sln)+butyl acetate(sln)=(*R*)-(+)-1-phenyl 1-butyl acetate(sln)+1-butanol(sln)

T/K	*K*
298.15	0.111

Reference: Tewari *et al.* (2003)[126]
Method: chromatography
Evaluation: A

Here "sln" refers to *n*-hexane.

(*R*)-(+)-1-phenyl ethanol(sln)+butyl acetate(sln)=(*R*)-(+)-1-phenyl ethyl acetate(sln)+1-butanol(sln)

T/K	Solvent	*K*
292.95	*n*-hexane	0.103
298.15	*n*-hexane	0.107
303.15	*n*-hexane	0.114
308.15	*n*-hexane	0.111
298.15	neat reaction mixture	0.294
298.15	carbon tetrachloride	0.112
298.15	acetonitrile	0.138
298.15	*tert*-butyl methyl ether	0.101
298.15	2-butanone	0.104

Reference: Tewari *et al.* (2003)[126]
Method: chromatography
Evaluation: A

Here "sln" refers to the several organic solvents used in this study. Tewari *et al.* calculated $\Delta_r G^\circ = 5.45$ kJ mol^{-1}, $\Delta_r H^\circ = 2.3$ kJ mol^{-1}, and $\Delta_r S^\circ = -11$ J K^{-1} mol^{-1} for this reaction carried out in *n*-hexane at $T = 298.15$ K.

(*R*)-(+)-1-phenyl-1-propanol(sln)+butyl acetate(sln)=(*R*)-(+)-1-phenyl-1-propyl acetate(sln)+1-butanol(sln)

T/K	*K*
298.15	0.105

Reference: Tewari *et al.* (2003)[126]
Method: chromatography
Evaluation: A

Here "sln" refers to *n*-hexane.

1,2,3-trioctanoyl glycerol(sln)+H_2O(sln)=1,2-dioctanoyl glycerol(sln)+*n*-octanoic acid(sln)

T/K	Solvent	*K*
310.15	acetonitrile	0.752
310.15	benzene	0.617
310.15	toluene	0.503
310.15	neat reaction mixture	1.75

Reference: Tewari and Bunk[109]
Method: chromatography
Evaluation: A

1,2,3-trioctanoyl glycerol(sln)+H_2O(sln)=1,3-dioctanoyl glycerol(sln)+*n*-octanoic acid(sln)

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T/K	Solvent	K
310.15	acetonitrile	1.11
310.15	benzene	0.91
310.15	toluene	0.74
310.15	neat reaction mixture	2.56

Reference: Tewari and Bunk[109]
Method: chromatography and mass spectrometry
Evaluation: A

1,2,3-trioctanoyl glycerol(sln)+3 H_2O(sln) = glycerol(sln)+3 *n*-octanoic acid(sln)

T/K	Solvent	K
310.15	acetonitrile	0.0610
310.15	benzene	0.645
310.15	toluene	0.444
310.15	neat reaction mixture	1.16

Reference: Tewari and Bunk[109]
Method: chromatography
Evaluation: A

1,2,3-trioctanoyl glycerol(sln)+2 H_2O(sln) = 1-monooctanoyl glycerol(sln)+2 *n*-octanoic acid(sln)

T/K	Solvent	K
310.15	acetonitrile	0.23
310.15	benzene	0.25
310.15	toluene	0.20
310.15	neat reaction mixture	1.75

Reference: Tewari and Bunk[109]
Method: chromatography
Evaluation: A

1,2,3-trioctanoyl glycerol(sln)+2 H_2O(sln) = 1-monooctanoyl glycerol(sln)+2 *n*-octanoic acid(sln)

T/K	Solvent	K
310.15	acetonitrile	0.12
310.15	benzene	0.13
310.15	toluene	0.10
310.15	neat reaction mixture	0.88

Reference: Tewari and Bunk[109]
Method: chromatography
Evaluation: A

4.49. Enzyme: alkaline phosphatase (EC 3.1.3.1)

cis-2-hydroxycyclopentanemethanol cyclic phosphate(aq) + H_2O(l) = *cis*-2-hydroxycyclopentanemethanol α-phosphate(aq)

T/K	pH	$\Delta_r H'^\circ$/(kJ mol^{-1})
298.15	7.3	−10.5

Reference: Gerlt *et al.* (1980)[46]
Method: calorimetry
Buffer: Pipes (0.05 mol dm^{-3})
pH: 7.3
Cofactor(s): Mg^{2+}
Evaluation: A

Gerlt *et al.* applied corrections for protonation of the buffer to obtain the value of $\Delta_r H'^\circ$ given here. An unclassified phosphorylase (EC 3.1.4.a) was also present.

trans-2-hydroxycyclopentanemethanol cyclic phosphate(aq) + H_2O(l) = *trans*-2-hydroxycyclopentanemethanol α-phosphate(aq)

T/K	pH	$\Delta_r H'^\circ$/(kJ mol^{-1})
298.15	7.3	−32.9

Reference: Gerlt *et al.* (1980)[46]
Method: calorimetry
Buffer: Pipes (0.05 mol dm^{-3})
pH: 7.3
Cofactor(s): Mg^{2+}
Evaluation: A

Gerlt *et al.* applied corrections for protonation of the buffer to obtain the value of $\Delta_r H'^\circ$ given here.

(1*R*,2*S*)-*trans*-2-hydroxytetrahydrofuranmethanol cyclic phosphate(aq) + H_2O(l) = (1*R*,2*S*)-*trans*-2-hydroxytetrahydrofuranmethanol α-phosphate(aq)

T/K	pH	$\Delta_r H'^\circ$/(kJ mol^{-1})
298.15	7.3	−44.2

Reference: Gerlt *et al.* (1980)[46]
Method: calorimetry
Buffer: Pipes (0.05 mol dm^{-3})
pH: 7.3
Cofactor(s): Mg^{2+}
Evaluation: A

Gerlt *et al.* applied corrections for protonation of the buffer to obtain the value of $\Delta_r H'^\circ$ given here.

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5-methoxytrimethylene phosphate(aq) + H_2O(l) = 2-methoxy-3-hydroxypropyl phosphate(aq)

T/K	pH	$\Delta_r H'^\circ$/(kJ mol^{-1})
298.15	7.3	−20.5

Reference: Gerlt *et al.* (1980)[46]
Method: calorimetry
Buffer: Pipes (0.05 mol dm^{-3})
pH: 7.3
Cofactor(s): Mg^{2+}
Evaluation: A

Gerlt *et al.* applied corrections for protonation of the buffer to obtain the value of $\Delta_r H'^\circ$ given here.

5-methyltrimethylene phosphate(aq) + H_2O(l) = 2-methyl-3-hydroxypropyl phosphate(aq)

T/K	pH	$\Delta_r H'^\circ$/(kJ mol^{-1})
298.15	7.3	−15.7

Reference: Gerlt *et al.* (1980)[46]
Method: calorimetry
Buffer: Pipes (0.05 mol dm^{-3})
pH: 7.3
Cofactor(s): Mg^{2+}
Evaluation: A

Gerlt *et al.* applied corrections for protonation of the buffer to obtain the value of $\Delta_r H'^\circ$ given here.

phospho*enol*pyruvate(aq) + H_2O(l) = pyruvate(aq) + orthophosphate(aq)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.62	0.33	−32.36

Reference: Goldberg and Tewari (2003)[120]
Method: calorimetry
Buffer: phosphate (0.10 mol kg^{-1})
pH: 7.62
Evaluation: A

Goldberg and Tewari also calculated $\Delta_r H^\circ$ = −29.8 kJ mol^{-1} at T = 298.15 K and I = 0 for the chemical reference reaction [phospho*enol*pyruvate^{3-}(aq) + H_2O(l) = pyruvate$^-$(aq) + HPO_4^{2-}(aq)].

4.50. Enzyme: 3′-5′-cyclic-nucleotide phosphodiesterase (EC 3.1.4.17)

adenosine 3′:5′-(cyclic)phosphate(aq) + H_2O(l) = AMP(aq)

T/K	pH	pMg	I_c/(mol dm^{-3})	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.53	4.20	0.32	−56.32

Reference: Goldberg and Tewari (2003)[120]
Method: calorimetry
Buffer: phosphate
pH: 7.53
Cofactor(s): $MgCl_2$ (0.0029 mol kg^{-1})
Evaluation: A

Goldberg and Tewari also calculated $\Delta_r H^\circ$ = −47.8 kJ mol^{-1} at T = 298.15 K and I = 0 for the chemical reference reaction [adenosine 3′:5′-(cyclic)phosphate$^-$(aq) + H_2O(l) = AMP$^-$(aq)].

4.51. Enzyme: 3′,5′-cyclic-GMP phosphodiesterase (EC 3.1.4.35)

guanosine 3′:5′-cyclic phosphate(aq) + H_2O(l) = guanosine 5′-phosphate(aq)

T/K	pH	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.15	−46.9

Reference: Hagins *et al.* (1989)[63]
Method: calorimetry
Buffer: Mops (0.010 mol dm^{-3})
pH: 7.15
Cofactor(s): $MgSO_4$ (0.0050 mol dm^{-3})
Evaluation: A

4.52. Enzyme: ADPglucose phosphodiesterase (EC 3.1.4.a)

(also see data given under alkaline phosphatase EC 3.1.3.1)

ADPglucose(aq) + H_2O(l) = α-**D**-glucose 1-phosphate(aq) + AMP(aq)

T/K	pH	K'_c
298.15	7.0	110

Reference: Rodriguez-Lopez *et al.* (2000)[104]
Method: spectrophotometry and chromatography
Buffer: Hepes (0.050 mol dm^{-3})
pH: 7.0
Cofactor(s): $MgCl_2$ (0.0050 mol dm^{-3})
Evaluation: C

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4.53. Enzyme: β-fructofuranosidase (EC 3.2.1.26)

sucrose(aq) + H_2O(l) = **D**-glucose(aq) + **D**-fructose(aq)

T/K	pH	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	4.94	−14.8

Reference: Rekharsky *et al.* (1994)[75]
Method: calorimetry
Buffer: acetate (0.10 mol dm^{-3})
pH: 4.94
Evaluation: A

sucrose(aq) + H_2O(l) = **D**-glucose(aq) + **D**-fructose(aq)

T/K	pH	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	4.6	−15.4

Reference: Hüttl *et al.* (1999)[90]
Method: calorimetry
Buffer: acetate (0.05 mol dm^{-3})
pH: 4.6
Cofactor(s): Cd^{2+}, Zn^{2+}, As^{3+}, As^{5+}, and Ag^{+}
Evaluation: B

4.54. Enzyme: inosine nucleosidase (EC 3.2.2.2)

inosine(aq) + H_2O(l) = hypoxanthine(aq) + **D**-ribose(aq)

T/K	pH	K'_c
310.15	7.5	106

Reference: Parkin *et al.* (1991)[67]
Method: chromatography
Buffer: Hepes (0.050 mol dm^{-3}) + NaOH
pH: 7.5
Evaluation: B

4.55. Enzyme: chymotripsin (EC 3.4.21.1)

4-nitrophenyl acetate(aq) + H_2O(l) = 4-nitrophenol(aq) + acetate(aq)

T/K	ϕ(acetonitrile)	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	1.6	−100
298.15	4.0	−106
298.15	10.0	−102

Reference: Sirotkin *et al.* (2005)[132]
Method: calorimetry and spectrophotometry
Buffer: Tris (0.033 mol dm^{-3}) + HCl
pH: 8.0
Evaluation: A

The quantity ϕ(acetonitrile) is the volume fraction of acetonitrile in the reaction mixture.

4.56. Enzyme: subtilisin (EC 3.4.21.62)

succinylAla-Ala-Pro-Leu-(4-nitrophenyl)analide(aq) + H_2O(l) = succinylAla-Ala-Pro-Leu(aq) + (4-nitrophenyl) analide(aq)

T/K	pH	$\Delta_r H$(cal)/(kJ mol^{-1})
295.15	8.6	−26.8

Reference: Williams and Toone (1994)[74]
Method: calorimetry
Buffer: Tris (0.10 mol dm^{-3}) + HCl
pH: 8.6
Evaluation: B

succinylAla-Ala-Pro-Phe-(4-nitrophenyl)analide(aq) + H_2O(l) = succinylAla-Ala-Pro-Phe(aq) + (4-nitrophenyl)analide(aq)

T/K	pH	$\Delta_r H$(cal)/(kJ mol^{-1})
295.15	8.6	−26.4

Reference: Williams and Toone (1994)[74]
Method: calorimetry
Buffer: Tris (0.10 mol dm^{-3}) + HCl
Evaluation: B

4.57. Enzyme: asparaginase(EC 3.5.1.1)

L-asparagine(aq) + H_2O(l) = **L**-aspartate(aq) + ammonia(aq)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.03	0.11	−25.63

Reference: Kishore *et al.* (2000)[101]
Method: calorimetry and chromatography
Buffer: potassium phosphate
pH: 7.03
Evaluation: A

Kishore *et al.* calculated $\Delta_r H^\circ = -26.17$ kJ mol^{-1} for the chemical reference reaction [**L**-asparagine(aq) + H_2O(l) = **L**-aspartate$^-$(aq) + NH_4^+(aq)] at $T = 298.15$ K and $I = 0$.

4.58. Enzyme: glutaminase (EC 3.5.1.2)

L-glutamine(aq) + H_2O(l) = **L**-glutamate(aq) + ammonia(aq)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	5.14	0.11	−24.39

Reference: Kishore *et al.* (2000)[101]
Method: calorimetry and chromatography
Buffer: potassium phosphate
pH: 5.14

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Evaluation: A

Kishore *et al.* calculated $\Delta_r H^\circ = -25.16$ kJ mol^{-1} for the chemical reference reaction [**L**-glutamine$^{\pm}$(aq) + H_2O(l) = **L**-glutamate$^-$(aq) + NH_4^+(aq)] at $T = 298.15$ K and $I = 0$.

4.59. Enzyme: penicillin amidase (EC 3.5.1.11)

amoxicillin(aq) + H_2O(l) = 6-aminopenicillanic acid(aq) + **D**-(4-hydroxyphenyl)glycine(aq)

T/K	pH	K'_c
298.15	5.1	1.85
298.15	5.1	2.09
298.15	5.6	8.06
298.15	5.6	6.67
298.15	5.6	4.83
298.15	6.0	20.4
298.15	6.0	15.0

Reference: Diender *et al.* (1998)[80]
Method: chromatography
Buffer: phosphate (0.1 mol dm^{-3})
pH: 5.1–6.0
Evaluation: A

The values of K' given here are shown in Fig. 2 of Diender *et al.* (1998).[80] The numerical values are based on a private communication from Straathof (2006).[141] The same results are given by Diender *et al.* (1998)[81] and by Diender (2000).[150]

cefamandole(aq) + H_2O(l) = 7-amino-3-((1-methyl-III-tetrazol-5-yl)-thiomethyl)-cephalosporanic acid(aq) + **D**-mandelic acid(aq)

T/K	pH	K'_c
283.15	4.25	0.023
303.15	4.25	0.029
303.15	3.00	0.0425
303.15	3.50	0.0283
303.15	3.76	0.0359
303.15	4.00	0.0300
303.15	4.28	0.0275
303.15	4.51	0.0417
303.15	5.02	0.0825

Reference: Nierstrsz *et al.* (1999)[93]
Method: chromatography
Buffer: phosphate
pH: 3.0–5.0
Evaluation: B

With the exception of the first two values given here, the values of K' were read from Fig. 5 of Nierstrsz *et al.* (1999).[93] Also, note that we have converted the reported values of K', given in units of mM, to a standard state of 1 mol dm^{-3}.

4.60. Enzyme: aminoacylase (EC 3.5.1.14)

2-acetamidohept-6-enoic acid(aq) + H_2O(l) = acetate(aq) + 2-aminohept-6-enoic acid(aq)

T/K	pH	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.5	−3.68

Reference: Williams and Toone (1994)[74]
Method: calorimetry
Buffer: phosphate (0.10 mol dm^{-3})
pH: 7.5
Evaluation: A

N-acetyl-**L**-alanine(aq) + H_2O(l) = acetate(aq) + **L**-alanine(aq)

T/K	pH	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.5	−4.85

Reference: Williams and Toone (1994)[74]
Method: calorimetry
Buffer: phosphate (0.10 mol dm^{-3})
pH: 7.5
Evaluation: A

N-acetyl-**L**-cysteine(aq) + H_2O(l) = acetate(aq) + **L**-cysteine(aq)

T/K	pH	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.5	−3.22

Reference: Williams and Toone (1994)[74]
Method: calorimetry
Buffer: phosphate (0.10 mol dm^{-3})
pH: 7.5
Evaluation: A

N-acetyl-**L**-methionine(aq) + H_2O(l) = acetate(aq) + **L**-methionine(aq)

T/K	*p*H	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.5	−2.34

Reference: Williams and Toone (1994)[74]
Method: calorimetry
Buffer: phosphate (0.10 mol dm^{-3})
pH: 7.5
Evaluation: A

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N-acetyl-**L**-norleucine(aq) + H_2O(l) = acetate(aq) + **L**-norleucine(aq)

T/K	pH	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.5	−3.47

Reference: Williams and Toone (1994)[74]
Method: calorimetry
Buffer: phosphate (0.10 mol dm^{-3})
pH: 7.5
Evaluation: A

N-acetyl-**L**-valine(aq) + H_2O(l) = acetate(aq) + **L**-valine(aq)

T/K	pH	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.5	−3.05

Reference: Williams and Toone (1994)[74]
Method: calorimetry
Buffer: phosphate (0.10 mol dm^{-3})
pH: 7.5
Evaluation: A

N-acetyl-**L**-phenylalanine(aq) + H_2O(l) = acetate(aq) + **L**-phenylalanine(aq)

T/K	pH	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.5	−2.76

Reference: Williams and Toone (1994)[74]
Method: calorimetry
Buffer: phosphate (0.10 mol dm^{-3})
pH: 7.5
Evaluation: A

4.61. Enzyme: anandamide amidohydrolase (EC 3.5.1.a)

anandamide(aq) + H_2O(l) = ethanolamine(aq) + arachidonic acid(aq)

T/K	pH	K'_c
310.15	6.0	1.5
310.15	7.4	0.41
310.15	9.0	0.22

Reference: Katayama *et al.* (1999)[91]
Method: radioactivity
Buffer: citrate (0.50 mol dm^{-3}) and [Tris (0.050 mol dm^{-3}) + HCl]
pH: 9.0
Evaluation: B

Katayama *et al.* reported ratios of c(arachidonic acid)/c(anandamode) with c(ethanolamine) fixed at 0.250 mol dm^{-3}. The values of K' given here were calculated by using these ratios and c(ethanolamine). Note that Katayama *et al.* also included $c(H_2O) = 55.5$ mol dm^{-3} in their reported values of K'.

palmitoylethanolamide(aq) + H_2O(l) = ethanolamine(aq) + palmitic acid(aq)

T/K	pH	K'_c
310.15	9.0	0.022

Reference: Katayama *et al.* (1999)[91]
Method: radioactivity
Buffer: Tris (0.050 mol dm^{-3}) + HCl
pH: 9.0
Evaluation: B

Katayama *et al.* reported the ratio of c(palmitic acid)/c(palmitoylethanolamide) with c(ethanolamine) fixed at 0.250 mol dm^{-3}. The value of K' given here was calculated by using these ratios and c(ethanolamine). Note that Katayama *et al.* also included $c(H_2O) = 55.5$ mol dm^{-3} in their reported value of K'.

4.62. Enzyme: dihydropyrimidinase (EC 3.5.2.2)

5,6-dihydrouracil(aq) + H_2O(l) = 3-ureidopropanoic acid(aq)

T/K	pH	I_m/(mol kg^{-1})	K'
298.15	6.80	0.28	25.9
298.15	7.38	0.31	64.8
298.15	7.84	0.32	160

Reference: Tewari *et al.* (2007)[148]
Method: chromatography
Buffer: phosphate
pH: 6.80–7.84
Evaluation: A

Tewari *et al.* also calculated $K = 2.3 \cdot 10^{-6}$ at $T = 298.15$ K and $I = 0$ for the chemical reference reaction [5,6-dihydrouracil(aq) + H_2O(l) = 3-ureidopropanoic acid$^-$(aq) + H^+(aq)].

5,6-dihydrouracil(aq) + H_2O(l) = 3-ureidopropanoic acid(aq)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.44	0.34	0.47

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Reference: Tewari *et al.* (2007)[148]
Method: chromatography
Buffer: phosphate
pH: 7.44
Evaluation: A

Tewari *et al.* also calculated $\Delta_r H^\circ = 5.9$ kJ mol^{-1} at $T = 298.15$ K and $I = 0$ for the chemical reference reaction [5,6-dihydrouracil(aq) + H_2O(l) = 3-ureidopropanoic acid$^-$(aq) + H^+(aq)].

hydantoin(aq) + H_2O(l) = ureidoacetic acid(aq)

T/K	pH	I_m/(mol kg^{-1})	K'
298.15	6.57	0.29	16.9
298.15	7.20	0.39	171

Reference: Tewari *et al.* (2007)[148]
Method: chromatography
Buffer: phosphate
pH: 6.57–7.20
Evaluation: A

Tewari *et al.* also calculated $K = 5.5 \cdot 10^{-6}$ at $T = 298.15$ K and $I = 0$ for the chemical reference reaction [hydantoin(aq) + H_2O(l) = ureidoacetic acid$^-$(aq) + H^+(aq)].

hydantoin(aq) + H_2O(l) = ureidoacetic acid(aq)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.39	0.37	−3.48

Reference: Tewari *et al.* (2007)[148]
Method: chromatography
Buffer: phosphate
pH: 7.39
Evaluation: A

Tewari *et al.* also calculated $\Delta_r H^\circ = 1.7$ kJ mol^{-1} at $T = 298.15$ K and $I = 0$ for the chemical reference reaction [hydantoin(aq) + H_2O(l) = ureidopropanoic acid$^-$(aq) + H^+(aq)].

5-(4-hydroxy)-phenylhydantoin(aq) + H_2O(l) = 5-(4-hydroxyphenyl) D-carbamoylate(aq)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.41	0.44	−3.7

Reference: Tewari *et al.* (2007)[148]
Method: chromatography
Buffer: phosphate
pH: 7.41
Evaluation: A

Tewari *et al.* also calculated $\Delta_r H^\circ = 8.7$ kJ mol^{-1} at $T = 298.15$ K and $I = 0$ for the chemical reference reaction [5-(4-hydroxyphenyl)hydantoin(aq) + H_2O(l) = 5-(4-hydroxyphenyl)**D**-carbamoylate(aq) + H^+(aq)].

5-(4-hydroxy)-phenylhydantoin(aq) + 3H_2O(l) = **D**-(4-hydroxyphenyl)glycine(aq) + carbon dioxide(aq) + ammonia(aq)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.41	0.42	−35.5

Reference: Tewari *et al.* (2007)[148]
Method: chromatography
Buffer: phosphate
pH: 7.41
Evaluation: A

Tewari *et al.* also calculated $\Delta_r H^\circ = -29.7$ kJ mol^{-1} at $T = 298.15$ K and $I = 0$ for the chemical reference reaction [5-(4-hydroxyphenyl)hydantoin(aq) + 3H_2O(l) = **D**-(4-hydroxyphenyl)glycine(aq) + HCO_3^-(aq) + NH_4^+(aq)].

5-phenylhydantoin(aq) + H_2O(l) = 5-phenyl D-carbamoylate(aq)

T/K	pH	$\frac{I_m}{\text{mol kg}^{-1}}$	K'
298.15	6.85	0.28	2.44
298.15	7.46	0.31	6.66
298.15	7.98	0.32	20.1

Reference: Tewari *et al.* (2007)[148]
Method: chromatography
Buffer: phosphate
pH: 6.85-7.98
Evaluation: A

Tewari *et al.* also calculated $K = 3.8 \cdot 10^{-7}$ at $T = 298.15$ K and $I = 0$ for the chemical reference reaction [5-phenylhydantoin(aq) + H_2O(l) = 5-phenyl **D**-carbamoylate$^-$(aq) + H^+(aq)].

5-phenylhydantoin(aq) + H_2O(l) = 5-phenyl D-carbamoylate(aq)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.42	0.32	−1.58

Reference: Tewari *et al.* (2007)[148]
Method: chromatography

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Buffer: phosphate
pH: 7.42
Evaluation: A

Tewari *et al.* also calculated $\Delta_r H^\circ = 10.8$ kJ mol^{-1} at $T = 298.15$ K and $I = 0$ for the chemical reference reaction [5-phenylhydantoin(aq) + H_2O(l) = 5-phenyl **D**-carbamoylate$^-$(aq) + H^+(aq)].

5-phenylhydantoin(aq) + $3H_2O$(l) = **D**-phenylglycine(aq) + carbon dioxide(aq) + ammonia(aq)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.48	0.37	−41.6

Reference: Tewari *et al.* (2007)[148]
Method: chromatography
Buffer: phosphate
pH: 7.48
Evaluation: A

Tewari *et al.* also calculated $\Delta_r H^\circ = -35.4$ kJ mol^{-1} at $T = 298.15$ K and $I = 0$ for the chemical reference reaction [5-phenylhydantoin(aq) + $3H_2O$(l) = **D**-phenylglycine(aq) + HCO_3^-(aq) + NH_4^+(aq)].

4.63. Enzyme: GTP cyclohydrolase I (EC 3.5.4.16)

GTP(aq) + H_2O(l) = ((2*R*,3*S*,4*R*,5*R*)-5-(2-amino-5-formamido-6-oxo-3,6-dihydropyrimidin-4-ylamino)-3,4-dihydroxytetrahydrofuran-2-yl)methyl tetrahydrogen triphosphate(aq)

T/K	pH	K'
303.15	7.0	0.1

Reference: Bracher *et al.* (1999)[87]
Method: spectrophotometry and NMR
Buffer: phosphate
pH: 7.0
Evaluation: B

The enzyme used is a mutant of GTP cyclohydrolase I. The value of K' is approximate.

4.64. Enzyme: nitrilase (EC 3.5.5.1)

benzonitrile(aq) + $2H_2O$(aq) = benzoic acid(aq) + ammonia(aq)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.51	0.29	−76.13

Reference: Tewari and Goldberg (2005)[133]
Method: calorimetry
Buffer: phosphate
pH: 7.5
Evaluation: A

Tewari and Goldberg calculated $\Delta_r H^\circ = -76.7$ kJ mol^{-1} for the chemical reference reaction [benzonitrile^0(aq) + $2H_2O$(l) = benzoate$^-$(aq) + NH_4^+(aq)] at $T = 298.15$ K and $I = 0$.

benzyl cyanide(aq) + $2H_2O$(aq) = phenylacetic acid(aq) + ammonia(aq)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.51	0.29	−88.06

Reference: Tewari and Goldberg (2005)[133]
Method: calorimetry
Buffer: phosphate
pH: 7.5
Evaluation: A

Tewari and Goldberg calculated $\Delta_r H^\circ = -89.0$ kJ mol^{-1} for the chemical reference reaction [benzyl cyanide^0(aq) + $2H_2O$(l) = benzeneacetate$^-$(aq) + NH_4^+(aq)] at $T = 298.15$ K and $I = 0$.

3-indoleacetonitrile(aq) + $2H_2O$(l) = indole-3-acetic acid(aq) + ammonia(aq)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.51	0.29	−97.61

Reference: Tewari and Goldberg (2005)[133]
Method: calorimetry
Buffer: phosphate
pH: 7.5
Evaluation: A

Tewari and Goldberg calculated $\Delta_r H^\circ = -99.0$ kJ mol^{-1} for the chemical reference reaction [3-indoleacetonitrile^0(aq) + $2H_2O$(l) = indole-3-acetate$^-$(aq) + NH_4^+(aq)] at $T = 298.15$ K and $I = 0$.

α-methylbenzylcyanide(aq) + $2H_2O$(l) = α-methylbenzene acetic acid(aq) + ammonia(aq)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.51	0.29	−82.59

Reference: Tewari and Goldberg (2005)[133]
Method: calorimetry
Buffer: phosphate
pH: 7.5
Evaluation: A

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Tewari and Goldberg calculated $\Delta_r H^\circ = -83.3$ kJ mol^{-1} for the chemical reference reaction [α-methylbenzylcyanide^0(aq) + 2H$_2$O(l) = α-methylbenzeneacetate$^-$(aq) + NH$_4^+$(aq)] at $T = 298.15$ K and $I = 0$.

4-phenylbutyronitrile(aq) + 2H$_2$O(l) = 4-phenylbutanoic acid(aq) + ammonia(aq)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.51	0.29	−81.03

Reference: Tewari and Goldberg (2005)[133]
Method: calorimetry
Buffer: phosphate
pH: 7.5
Evaluation: A

Tewari and Goldberg calculated $\Delta_r H^\circ = -82.0$ kJ mol^{-1} for the chemical reference reaction [4-phenylbutyronitrile^0(aq) + 2H$_2$O(l) = 4-phenylbutyrate$^-$(aq) + NH$_4^+$(aq)] at $T = 298.15$ K and $I = 0$.

3-phenylpropionitrile(aq) + 2H$_2$O(l) = 3-phenylpropanoic acid(aq) + ammonia(aq)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.51	0.29	−90.73

Reference: Tewari and Goldberg (2005)[133]
Method: calorimetry
Buffer: phosphate
pH: 7.5
Evaluation: A

Tewari and Goldberg calculated $\Delta_r H^\circ = -91.3$ kJ mol^{-1} for the chemical reference reaction [3-phenylpropionitrile^0(aq) + 2H$_2$O(l) = 3-phenylpropanoate$^-$(aq) + NH$_4^+$(aq)] at $T = 298.15$ K and $I = 0$.

4.65. Enzyme: inorganic pyrophosphatase (EC 3.6.1.1)

pyrophosphate(aq) + H$_2$O(l) = 2 orthophosphate(aq)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_r H$(cal)/(kJ mol^{-1})
303.15	7.5	0	−27.6
303.15	7.5	0.10	−26.4

Reference: da-Silva *et al.* (2004)[128]
Method: calorimetry
Buffer: Mops + Tris
pH: 7.5
Cofactor(s): $MgCl_2$ (0.0006 mol dm^{-3})
Evaluation: A

da-Silva *et al.* also performed calorimetric measurements in which a membrane-bound inorganic pyrophosphatase was used.

4.66. Enzyme: adenosinetriphosphatase (EC 3.6.1.3)

ATP(aq) + H$_2$O(l) = ADP(aq) + orthophosphate(aq)

T/K	pH	$\Delta_r H$(cal)/(kJ mol^{-1})
310.15	7.4	−40.41

Reference: Li *et al.* (2004)[129]
Method: calorimetry
Buffer: Tris (0.10 mol dm^{-3}) + HCl
pH: 7.4
Cofactor(s): $MgCl_2$
Evaluation: A

4.67. Enzyme: inosine triphosphate pyrophosphohydrolase (EC 3.6.1.a)

ITP(aq) + H$_2$O(l) = IMP(aq) + pyrophosphate(aq)

T/K	pH	K'_c
303.15	8.5	$3.8 \cdot 10^4$

Reference: Vanderheiden (1979)[44]
Method: radioactivity
Buffer: glycine (0.050 mol dm^{-3})
pH: 8.5
Cofactor(s): $MgCl_2$ (0.050 mol dm^{-3})
Evaluation: C

4.68. Enzyme: oxaloacetate decarboxylase (EC 4.1.1.3)

oxaloacetate(aq) = pyruvate(aq) + carbon dioxide(aq)

T/K	pH	K'_c
298.15	7.0	0.47

Reference: Ng *et al.* (1982)[48]
Method: spectrophotometry and enzymatic assay
Buffer: phosphate (0.005 mol dm^{-3})
pH: 7.0
Cofactor(s): Mg^{2+} (0.005 mol dm^{-3})
Evaluation: C

The value of K'_c given here was calculated from the concentrations of the reactants and products reported by Ng *et al.*

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4.69. Enzyme: orotidine-5′-phosphate decarboxylase (EC 4.1.1.23)

orotidine 5′-phosphate(aq)=UMP(aq)
+carbon dioxide(aq)

T/K	pH	$\Delta_r H$(cal)/(kJ mol^{-1})
328.15	7.5	−20.92

Reference: Poduch *et al.* (2006)[140]
Method: calorimetry
Buffer: Tris (0.050 mol dm^{-3})
pH: 7.5
Evaluation: B

$\Delta_r H$(cal) for this reaction is exothermic [Kotra (2007)[146]].

4.70. Enzyme: ribulose-bisphosphate carboxylase (EC 4.1.1.39)

D-ribulose1,5-bisphosphate(aq)+carbon dioxide(aq)
=23-phospho-**D**-glycerate(aq)

T/K	pH	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	8.0	−62.3

Reference: Frank *et al.* (2000)[100]
Method: calorimetry
Buffer: Tris (0.10 mol dm^{-3})+HCl
pH: 8.0
Cofactor(s): Mg^{2+} (0.010 mol dm^{-3})
Evaluation: A

D-ribulose1,5-bisphosphate(aq)+O_2(aq)=3-phospho-**D**-glycerate(aq)

T/K	pH	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	8.0	−401

Reference: Frank *et al.* (2000)[100]
Method: calorimetry
Buffer: Tris (0.10 mol dm^{-3})+HCl
pH: 8.0
Cofactor(s): Co^{2+} (0.010 mol dm^{-3})
Evaluation: A

4.71. Enzyme: deoxyribose-phosphate aldolase (EC 4.1.2.4)

2-deoxy-D-ribose 5-phosphate(aq)=**D**-glyceraldehyde 3-phosphate(aq)+acetaldehyde(aq)

T/K	pH	K'_c
298.15	7.0	$2.4\cdot10^{-4}$

Reference: Tischer *et al.* (2001)[111]
pH: 7.0
Evaluation: C

Few experimental details are given in this patent. The temperature is assumed to be 298.15 K.

4.72. Enzyme: fructose-bisphosphate aldolase (EC 4.1.2.13)

D-fructose 1,6-bisphosphate(aq)
=glycerone phosphate(aq)
+**D**-glyceraldehyde 3-phosphate(aq)

T/K	K'_c
298.15	$1.0\cdot10^{-4}$

Reference: Tischer *et al.* (2001)[111]
Evaluation: C

Few experimental details are given in this patent. The temperature is assumed to be 298.15 K. The pH was not reported.

4.73. Enzyme: 2-dehydro-3-deoxyheptonate aldolase (EC 4.1.2.15)

phospho*enol*pyruvate(aq)+**D**-erythrose 4-phosphate(aq)
+H_2O(l)=2-dehydro-3-deoxy-**D**-arabino-heptonate 7
-phosphate(aq)+orthophosphate(aq)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	8.18	0.090	−67.7

Reference: Tewari *et al.* (2001)[110]
Method: calorimetry
Buffer: Tris+HCl
pH: 8.18
Cofactor(s): $MnCl_2$
Evaluation: A

Tewari *et al.* also calculated $\Delta_r H^\circ = -70.0$ kJ mol^{-1} at T =298.15 K and I=0 for the chemical reference reaction [phospho*enol*pyruvate^{3-}(aq)+**D**-erythrose 4-phosphate^{2-}(aq)
+H_2O(l)=2-dehydro-3-deoxy-**D**-arabino-heptonate 7-phosphate^{3-}(aq)+HPO_4^{2-}(aq)].

4.74. Enzyme: 2-oxo-3-deoxy-D-gluconate aldolase (EC 4.1.2.a)

2-oxo-3-deoxy-**D**-gluconate(aq)=pyruvate(aq)
+**D**-glyceraldehyde(aq)

T/K	pH	K'_c
313.15	8.0	$8.8\cdot10^{-4}$

Reference: Elsayed (1999)[88]

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Method: spectrophotometry and enzymatic assay
Buffer: Tris+HCl
pH: 8.0
Evaluation: C

4.75. Enzyme: isocitrate lyase (EC 4.1.3.1)

isocitrate(aq)=succinate(aq)+glyoxylate(aq)

T/K	pH	K'_c
295.65	7.0	870

Reference: Ranaldi *et al.* (2003)[124]
Method: spectrophotometry.
Buffer: Hepes (0.066 mol dm^{-3})
pH: 7.0
Cofactor(s): $MgCl_2$ (0.0060 mol dm^{-3})
Evaluation: B

The equilibrium constant was calculated by using the Haldane relation. Experiments were conducted both at microgravity ($\sim$0 g_n) and at standard gravity (1 g_n). The value of K' given here is the average of these two results.

4.76. Enzyme: anthranilate synthase (EC 4.1.3.27)

chorismate(aq)+ammonia(aq)
=2-amino-2-deoxyisochorismate(aq)+H_2O(l)

T/K	pH	I_m/(mol kg^{-1})	K'_m
288.15	8.08	0.15	9.50
293.15	8.00	0.15	9.02
298.15	7.86	0.14	8.44
302.75	7.76	0.14	7.51

Reference: Byrnes *et al.* (2000)[97]
Method: calorimetry, spectrophotometry, and chromatography
Buffer: Tricine+NaOH
pH: 7.76–8.00
Cofactor(s): $MgCl_2$
Evaluation: A

Byrnes *et al.* also calculated K=20.3 and $\Delta_r H^\circ$=−10.5 kJ mol^{-1} at T=298.15 K and I=0 for the chemical reference reaction [chorismate^{2-}(aq)+NH_4^+(aq)=2-amino-2-deoxyisochorismate$^-$(aq)+H_2O(l)].

chorismate(aq)+ammonia(aq)=anthranilate(aq)
+pyruvate(aq)+H_2O(l)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.79	0.56	−123.7

Reference: Byrnes *et al.* (2000)[97]
Method: calorimetry, spectrophotometry, and chromatography
Buffer: phosphate
pH: 7.79
Cofactor(s): $MgCl_2$ (0.0017 mol dm^{-3})
Evaluation: A

Byrnes *et al.* also calculated $\Delta_r H^\circ$=−116.3 kJ mol^{-1} at T=298.15 K and I=0 for the chemical reference reaction [chorismate^{2-}(aq)+NH_4^+(aq)=anthranilate$^-$(aq)+pyruvate$^-$(aq)+H_2O(l)+H^+(aq)].

4.77. Enzyme: 3-dehydroquinate dehydratase (EC 4.2.1.10)

3-dehydroquinate(aq)=3-dehydroshikimate(aq)+H_2O(l)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	7.42	0.069	2.3

Reference: Tewari *et al.* (2002)[117]
Method: calorimetry
Buffer: Hepes+NaOH
pH: 7.42
Cofactor(s): NAD(ox) and Zn^{2+}(aq)
Evaluation: A

4.78. Enzyme: enoyl-CoA hydratase (EC 4.2.1.17)

(3*S*)-hydroxybutanoyl-coenzyme A(aq)
=*trans*-but-2-enoyl-coenzyme A+H_2O(l)

T/K	pH	K'
298.15	7.4	0.13

Reference: Wu *et al.* (2000)[151]
Method: NMR
Buffer: phosphate (0.020 mol dm^{-3})
pH: 7.4
Evaluation: A

Wu *et al.* also estimated $K' \approx 10^{-3}$ for the reaction [(3*R*)-hydroxybutanoyl-CoA(aq)=*cis*-but-2-enoyl-coenzyme A(aq)+H_2O(1)] at T=298.15 K and pH=7.4.

4.79. Enzyme: carnitine dehydratase (EC 4.2.1.89)

L-carnitine(aq)=4-(trimethylammonio)but-2-enoate(aq)
+H_2O(l)

T/K	pH	K'
310.15	7.8	1.5

Reference: Jung *et al.* (1989)[64]
Method: radioactivity
Buffer: potassium phosphate (0.05 mol dm^{-3})
pH: 7.8

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Evaluation: A

4.80. Enzyme: 3-dehydroquinate synthase (EC 4.6.1.3)

2-dehydro-3-deoxy-D-arabino-heptonate 7-phosphate(aq) = 3-dehydroquinate(aq) + orthophosphate(aq)

T/K	pH	I_m/(mol kg^{-1})	K'_m
298.15	7.50	0.065	4.6

Reference: Tewari *et al.* (2002)[117]
Method: chromatography
Buffer: Hepes + NaOH
pH: 7.5
Cofactor(s): NAD(ox) and Zn^{2+}(aq)
Evaluation: A

2-dehydro-3-deoxy-D-arabino-heptonate 7-phosphate(aq) = 3-dehydroquinate(aq) + orthophosphate(aq)

T/K	pH	pMn	I_m/(mol kg^{-1})	$\Delta_t H$(cal)/(kJ mol^{-1})
298.15	7.46	3.30	0.070	−50.9

Reference: Tewari *et al.* (2002)[117]
Method: calorimetry
Buffer: Hepes + NaOH
pH: 7.5
Cofactor(s): NAD(ox) and Zn^{2+}(aq)
Evaluation: A

The quantity pMn = −lg[m(Mn^{2+})].

4.81. Enzyme: alanine racemase (EC 5.1.1.1)

L-alanine(aq) = **D**-alanine(aq)

T/K	pH	K'
310.15	9.2	1.01

Reference: Wasserman *et al.* (1984)[52]
Method: spectrophotometry
Buffer: Ches (0.10 mol dm^{-3})
pH: 9.0
Evaluation: C

The value of K' was obtained by using the Haldane relation. The value of this equilibrium constant must equal unity.

L-alanine(aq) = **D**-alanine(aq)

T/K	pH	K'
310.15	9.0	0.8

Reference: Badet and Walsh (1985)[53]
Method: spectrophotometry
Buffer: Ches (0.10 mol dm^{-3})
pH: 9.0
Evaluation: C

The value of this equilibrium constant must equal 1.0.

L-alanine(aq) = **D**-alanine(aq)

T/K	pH	K'
310.15	9.0	0.8

Reference: Watanabe *et al.* (2003)[127]
Method: chromatography
Buffer: Bis-tris propane (0.10 mol dm^{-3})
pH: 9.0
Evaluation: C

The value of K' was obtained by using the Haldane relation. The value of this equilibrium constant must equal unity.

L-alanine(aq) = **D**-alanine(aq)

T/K	pH	K'
310.15	9.0	1.0

Reference: Ono *et al.* (2006)[139]
Method: chromatography
Buffer: Ches (0.010 mol dm^{-3})
pH: 9.0
Evaluation: B

The value of this equilibrium constant must equal unity.

4.82. Enzyme: UDPglucose 4-epimerase (EC 5.1.3.2)

UDP-*N*-acetyl-**D**-glucosamine(aq) = UDP-*N*-acetyl-**D**-galactosamine(aq)

T/K	K'
310.15	0.38

Reference: Piller *et al.* (1983)[49]
Method: radioactivity
Buffer: Tris + HCl
Evaluation: C

The temperature is assumed to be that used for their enzyme assays. The pH at which the equilibrium measurements were performed was not reported by Piller *et al.*

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UDPglucose(aq)=UDPgalactose(aq)

T/K	K'
310.15	0.38

Reference: Piller *et al.* (1983)[49]
Method: radioactivity
Buffer: Tris (0.050 mol dm^{-3})+HCl
Evaluation: C

The temperature is assumed to be that used for their enzyme assays. The pH at which the equilibrium measurements were performed was not reported by Piller *et al.*

4.83. Enzyme: UDPglucuronate 4-epimerase (EC 5.1.3.6)

UDP-**D**-glucuronate(aq)=UDP-**D**-galacturonate(aq)

T/K	pH	K'
310.15	7.5	1.3

Reference: Munoz *et al.* (1999)[92]
Method: chromatography
Buffer: Tris (0.050 mol dm^{-3})+HCl
pH: 7.5
Evaluation: B

4.84. Enzyme: dTDP-4-dehydrorhamnose 3,5-epimerase (EC 5.1.3.13)

4.85. Enzyme: xylose isomerase (EC 5.3.1.5)

D-arabinose(aq)=**D**-ribose(aq)

T/K	pH	K'
298.15	7.2	0.22
313.15	7.2	0.30
323.15	7.2	0.32
333.15	7.2	0.37
343.15	7.2	0.40

Reference: Vuolanto *et al.* (2002)[118]
Method: chromatography
Buffer: maleate (0.050 mol dm^{-3})
pH: 7.2
Evaluation: C

The values of K' given here were calculated from the concentrations reported by Vuolanto *et al.* Both the **D**- and **L**-forms of arabinose and ribose were used as starting material.

D-arabinose(aq)=**D**-ribulose(aq)

T/K	pH	K'
298.15	7.2	0.038
313.15	7.2	0.067
323.15	7.2	0.085
333.15	7.2	0.12
343.15	7.2	0.14

Reference: Vuolanto *et al.* (2002)[118]
Method: chromatography
Buffer: maleate (0.050 mol dm^{-3})
pH: 7.2
Evaluation: C

The values of K' given here were calculated from the concentrations reported by Vuolanto *et al.* Both the **D**- and **L**-forms of arabinose were used as starting material.

D-erythrose(aq)=**D**-erythrulose(aq)

T/K	pH	K'
298.15	7.2	2.04
313.15	7.2	2.30
323.15	7.2	2.73
333.15	7.2	2.67
343.15	7.2	3.00

Reference: Vuolanto *et al.* (2002)[118]
Method: chromatography
Buffer: maleate (0.050 mol dm^{-3})
pH: 7.2
Evaluation: C

The values of K' given here were calculated from the concentrations reported by Vuolanto *et al.* Both the **D**- and **L**-forms of erythrose were used as starting material. We calculate $\Delta_r H'^\circ = -1.8$ kJ mol^{-1} at $T=298.15$ K for this reaction from the temperature dependence of the K' values.

D-erythrose(aq)=**D**-threose(aq)

T/K	pH	K'
298.15	7.2	0.96
313.15	7.2	1.04
323.15	7.2	0.82
333.15	7.2	1.10
343.15	7.2	0.76

Reference: Vuolanto *et al.* (2002)[118]
Method: chromatography
Buffer: maleate (0.050 mol dm^{-3})
pH: 7.2
Evaluation: C

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The values of K' given here were calculated from the concentrations reported by Vuolanto *et al.* Both the D- and L-forms of erythrose and threose were used as starting material.

D-glucose(aq) = **D**-fructose(aq)

T/K	pH	K'
333.15	7.0	0.99
338.15	7.0	1.02
343.15	7.0	1.14
348.15	7.0	1.21
353.15	7.0	1.39

Reference: Converti and Del Borghi (1998)[79]
Method: chromatography
Buffer: Tris (0.05 mol dm^{-3}) + HCl
pH: 7.0
Cofactor(s): $MgSO_4$
Evaluation: B

The results were obtained from the analysis of kinetic data (Haldane relation). The K' values given here were obtained from Fig. 2 of Converti and Del Borghi. We calculate $\Delta_r H'^\circ = 16.6$ kJ mol^{-1} at $T = 298.15$ K for this reaction from the temperature dependence of the K' values.

D-glucose(aq) = **D**-fructose(aq)

T/K	pH	K'
333.15	7.2	1.03

Reference: Vuolanto *et al.* (2002)[118]
Method: chromatography
Buffer: maleate (0.050 mol dm^{-3})
pH: 7.2
Evaluation: C

The value of K' given here was calculated from the concentrations reported by Vuolanto *et al.* Both the D- and L-forms of glucose were used as starting material.

D-glucose(aq) = **D**-mannose(aq)

T/K	pH	K'
333.15	7.2	0.48

Reference: Vuolanto *et al.* (2002)[118]
Method: chromatography
Buffer: maleate (0.050 mol dm^{-3})
pH: 7.2
Evaluation: C

The value of K' given here was calculated from the concentrations reported by Vuolanto *et al.* Both the D- and L-forms of glucose and mannose were used as starting material.

4.86. Enzyme: glucose-6-phosphate isomerase (EC 5.3.1.9)

D-glucose 6-phosphate(aq) = **D**-fructose 6-phosphate(aq)

T/K	pH	$c(MgCl_2)$/(mol dm^{-3})	K'
293.4	8.0	0.10	0.307
298.4	8.0	0.10	0.395

Reference: Stödeman and Schwarz (2004)[130]
Method: calorimety
Buffer: Tris (0.10 mol dm^{-3}) + HCl
pH: 8.0
Cofactor(s): $MgCl_2$
Evaluation: A

D-glucose 6-phosphate(aq) = **D**-fructose 6-phosphate(aq)

T/K	pH	$c(MgCl_2)$/(mol dm^{-3})	K'
293.4	8.0	0.10	7.64
298.15	8.0	0.10	11.7
298.4	8.0	0.10	8.16
303.4	8.0	0.10	8.13
311.5	8.0	0.10	8.96

Reference: Stödeman and Schwarz (2004)[130]
Method: calorimetry
Buffer: Tris (0.10 mol dm^{-3}) + HCl
pH: 8.0
Cofactor(s): $MgCl_2$
Evaluation: A

The values for $\Delta_r H$(cal) at $T = 293.4$ K and at $T = 298.4$ K are the averages of the values of $\Delta_r H$(cal) reported in Table 4 of Stödeman and Schwarz (2004).[130]

4.87. Enzyme: arabinose-5-phosphate isomerase (EC 5.3.1.13)

D-arabinose 5-phosphate(aq) = **D**-ribulose 5-phosphate(aq)

T/K	pH	K'
310.15	7.5	0.50

Reference: Meredith and Woodard (2003)[123]
Method: NMR
Buffer: Tris (0.50 mol dm^{-3}) + HCl
pH: 7.5
Evaluation: B

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The authors also used the Haldane relation to calculate $K'=0.35$.

4.88. Enzyme: cholestenol Δ-isomerase (EC 5.3.3.5)

$(3\beta,5\alpha)$-cholesta-7,24-diene-3-ol(aq) = $(3\beta,5\alpha)$-cholesta-8,24-diene-3-ol(aq)

T/K	pH	K'
310.15	7.5	14

Reference: Nes *et al.* (2002)[116]
Method: chromatography and radioactivity
Buffer: Tris (0.05 mol dm^{-3}) + HCl
pH: 7.5
Evaluation: C

This result is based on kinetic data (Haldane relation).

4.89. Enzyme: phosphoglycerate mutase (EC 5.4.2.1)

2-phospho-**D**-glycerate(aq) = 3-phospho-**D**-glycerate(aq)

T/K	pH	$c(Mg^{2+})$/(mol dm^{-3})	K'
298.15	7.4	0	11.9

Reference: Britton and Clarke (1971)[36]
Method: radioactivity
Buffer: Tris
pH: 7.4
Evaluation: C

This result by Britton and Clarke (1971)[36] is cited as unpublished data by Britton *et al.* (1971).[35] The temperature is assumed to be 298.15 K. Clarke *et al.* (1974)[37] later reported a detailed study of the apparent equilibrium constant for this reaction.

2-phospho-**D**-glycerate(aq) = 3-phospho-**D**-glycerate(aq)

T/K	pH	K'
298.15	7.5	12.7

Reference: Rose and Dube (1978)[43]
Method: radioactivity
Buffer: Tes (0.050 mol dm^{-3})
pH: 7.5
Cofactor(s):
Evaluation: C

2-phospho-**D**-glycerate(aq) = 3-phospho-**D**-glycerate(aq)

T/K	pH	K'
298.15	7.4	2.8

Reference: Gautan (1988)[61]
Method: spectrophotometry
Buffer: triethanolamine (0.050 mol dm^{-3})
pH: 7.4
Cofactor(s): $MgCl_2$ (0.010 mol dm^{-3})
Evaluation: B

This approximate result is the average of the results obtained with two different varieties of this enzyme and is based on kinetic data (Haldane relation). The conditions of measurement were not reported. The temperature is assumed to be ~298.15 K.

4.90. Enzyme: phospho*enol*pyruvate mutase (EC 5.4.2.9)

phospho*enol*pyruvate(aq) = 3-phosphonopyruvate(aq)

T/K	pH	K'
298.15	7.5	$8\cdot10^{-4}$

Reference: Kim and Dunaway-Mariano[77]
Method: spectrophotometry
Buffer: Hepes (0.50 mol dm^{-3})
pH: 7.5
Cofactor(s): $MgCl_2$ (0.0050 mol dm^{-3})
Evaluation: B

Kim and Dunaway-Mariano also obtained a value of $K'=2\cdot10^{-4}$ from kinetic data (Haldane relation).

4.91. Enzyme: isochorismate synthase (EC 5.4.99.6)

chorismate(aq) = isochorismate(aq)

T/K	pH	I_m/(mol kg^{-1})	K'
298.15	7.34	0.31	0.84

Reference: Tewari *et al.* (2000)[106]
Method: chromatography
Buffer: potassium phosphate (0.10*M*)
pH: 7.34
Cofactor(s): $MgCl_2$
Evaluation: A

Tewari *et al.* calculated $K=0.84$, $\Delta_rG^\circ=0.43$ kJ mol^{-1}, $\Delta_rH^\circ=-0.81$ kJ mol^{-1}, and $\Delta_rS^\circ=-4.2$ J K^{-1} mol^{-1} for the chemical reference reaction [chorismate^{2-}(aq) = isochorismate^{2-}(aq)] at $T=298.15$ K and $I=0$.

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chorismate(aq) = isochorismate(aq)

T/K	pH	I_m/(mol kg^{-1})	$\Delta_r H$(cal)/(kJ mol^{-1})
298.15	6.93	0.23	−0.81

Reference: Tewari *et al.* (2000)[106]
Method: calorimetry and chromatography
Buffer: potassium phosphate (0.10*M*)
pH: 6.93
Cofactor(s): $MgCl_2$
Evaluation: A

Tewari *et al.* calculated $K = 0.84$, $\Delta_r G^\circ = 0.43$ kJ mol^{-1}, $\Delta_r H^\circ = -0.81$ kJ mol^{-1}, and $\Delta_r S^\circ = -4.2$ J K^{-1} mol^{-1} for the chemical reference reaction [chorismate^{2-}(aq) = isochorismate^{2-}(aq)] at $T = 298.15$ K and $I = 0$.

4.92. Enzyme: tyrosine-tRNA ligase (EC 6.1.1.1)

ATP(aq) + L-tyrosine(aq) + tRNA^{Tyr}(aq) = AMP(aq) + pyrophosphate(aq) + L-tyrosyl-tRNA^{Tyr}(aq)

T/K	pH	$c(Mg^{2+})$/(mol dm^{-3})	c(spermidine)/(mol dm^{-3})	K'
303.15	7.4	0.000 32	0	0.91
303.15	7.4	0.000 32	0.001	0.95
303.15	7.4	0.000 66	0	0.96
303.15	7.4	0.000 66	0.001	0.98
303.15	7.4	0.0011	0	0.96
303.15	7.4	0.0011	0.001	1.09
303.15	7.4	0.0020	0	1.07
303.15	7.4	0.0020	0.001	1.09
303.15	7.4	0.0030	0	1.21
303.15	7.4	0.0030	0.001	1.21
303.15	7.4	0.0040	0	1.31
303.15	7.4	0.0040	0.001	1.35
303.15	7.4	0.0060	0	1.56
303.15	7.4	0.0060	0.001	1.80
303.15	7.4	0.010	0	1.99
303.15	7.4	0.010	0.001	2.16
303.15	7.4	0.014	0	2.69
303.15	7.4	0.014	0.001	2.46
303.15	7.4	0.018	0	3.03
303.15	7.4	0.018	0.001	2.91

Reference: Airas (2007)[152]
Method: radioactivity
Buffer: Hepes (0.050 mol dm^{-3}) + KOH
pH: 7.4
Cofactor(s): $Mg(acetate)_2$
Evaluation: A

4.93. Enzyme: threonin-tRNA ligase (EC 6.1.1.3)

ATP(aq) + L-threonine(aq) + tRNA^{Thr}(aq) = AMP(aq) + pyrophosphate(aq) + L-threonyl-tRNA^{Thr}(aq)

T/K	pH	K'
310.16	7.0	0.37

Reference: Leahy *et al.* (1960)[32]
Method: radioactivity
Buffer: Tris
pH: 7.0
Cofactor(s): Mg^{2+}
Evaluation: B

4.94. Enzyme: isoleucine-tRNA ligase (EC 6.1.1.5)

ATP(aq) + L-isoleucine(aq) + tRNA^{Ile}(aq) = AMP(aq) + pyrophosphate(aq) + L-isoleucyl-tRNA^{Ile}(aq)

T/K	pH	$c(Mg^{2+})$/(mol dm^{-3})	c(spermidine)/(mol dm^{-3})	K'
303.15	7.4	0.000 60	0	0.45
303.15	7.4	0.000 60	0.001	0.54
303.15	7.4	0.0015	0	0.56
303.15	7.4	0.0015	0.001	0.61
303.15	7.4	0.0025	0	0.63
303.15	7.4	0.0025	0.001	0.65
303.15	7.4	0.0035	0	0.69
303.15	7.4	0.0035	0.001	0.72
303.15	7.4	0.0055	0	0.83
303.15	7.4	0.0055	0.001	0.80
303.15	7.4	0.0075	0	0.94
303.15	7.4	0.0075	0.001	0.92
303.15	7.4	0.0095	0	1.04
303.15	7.4	0.0095	0.001	1.02
303.15	7.4	0.0135	0	1.22
303.15	7.4	0.0135	0.001	1.17
303.15	7.4	0.0175	0	1.29
303.15	7.4	0.0175	0.001	1.28

Reference: Airas (2007)[152]
Method: radioactivity
Buffer: Hepes (0.050 mol dm^{-3}) + KOH
pH: 7.4
Cofactor(s): $Mg(acetate)_2$
Evaluation: A

4.95. Enzyme: lysine-tRNA ligase (EC 6.1.1.6)

ATP(aq) + L-lysine(aq) + tRNA^{Lys}(aq) = AMP(aq) + pyrophosphate(aq) + L-lysyl-tRNA^{Lys}(aq)

T/K	pH	$c(Mg^{2+})$/(mol dm^{-3})	c(spermidine)/(mol dm^{-3})	K'
303.15	7.4	0.000 60	0	0.85
303.15	7.4	0.000 60	0.001	1.16
303.15	7.4	0.0015	0	1.17
303.15	7.4	0.0015	0.001	1.22
303.15	7.4	0.0025	0	1.31

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T/K	pH	$c(Mg^{2+})$ / (mol dm^{-3})	c(spermidine) / (mol dm^{-3})	K'
303.15	7.4	0.0025	0.001	1.33
303.15	7.4	0.0035	0	1.43
303.15	7.4	0.0035	0.001	1.46
303.15	7.4	0.0055	0	1.68
303.15	7.4	0.0055	0.001	1.67
303.15	7.4	0.0075	0	1.92
303.15	7.4	0.0075	0.001	1.90
303.15	7.4	0.0095	0	2.05
303.15	7.4	0.0095	0.001	1.98
303.15	7.4	0.0135	0	2.34
303.15	7.4	0.0135	0.001	2.40
303.15	7.4	0.0175	0	2.63
303.15	7.4	0.0175	0.001	2.72

Reference: Airas (2007)[152]
Method: radioactivity
Buffer: Hepes (0.050 mol dm^{-3}) + KOH
pH: 7.4
Cofactor(s): $Mg(acetate)_2$
Evaluation: A

4.96. Enzyme: serine-tRNA ligase (EC 6.1.1.11)

ATP(aq) + L-serine(aq) + $tRNA^{Ser}$(aq) = AMP(aq) + pyrophosphate(aq) + L-seryl-$tRNA^{Ser}$(aq)

T/K	pH	$c(Mg^{2+})$ / (mol dm^{-3})	c(spermidine) / (mol dm^{-3})	K'
303.15	7.4	0.0010	0	0.54
303.15	7.4	0.0010	0.001	0.52
303.15	7.4	0.0020	0	0.60
303.15	7.4	0.0020	0.001	0.57
303.15	7.4	0.0030	0	0.73
303.15	7.4	0.0030	0.001	0.70
303.15	7.4	0.0060	0	1.00
303.15	7.4	0.0060	0.001	0.91
303.15	7.4	0.0010	0	1.34
303.15	7.4	0.0010	0.001	1.35
303.15	7.4	0.0014	0	1.69
303.15	7.4	0.0014	0.001	1.62
303.15	7.4	0.0018	0	2.13
303.15	7.4	0.0018	0.001	1.66

Reference: Airas (2006)[137]
Method: radioactivity
Buffer: Hepes (0.050 mol dm^{-3}) + KOH
pH: 7.4
Cofactor(s): $Mg(acetate)_2$
Evaluation: A

4.97. Enzyme: arginine-tRNA ligase (EC 6.1.1.19)

ATP(aq) + L-arginine(aq) + $tRNA^{Arg}$(aq) = AMP(aq) + pyrophosphate(aq) + L-arginyl-$tRNA^{Arg}$(aq)

T/K	pH	$c(Mg^{2+})$ / (mol dm^{-3})	c(spermidine) / (mol dm^{-3})	K'
303.15	7.4	0.000 60	0	0.97
303.15	7.4	0.000 60	0.001	1.05
303.15	7.4	0.001 0	0	1.28
303.15	7.4	0.0010	0.001	1.14
303.15	7.4	0.0020	0	1.40
303.15	7.4	0.0020	0.001	1.17
303.15	7.4	0.0030	0	1.43
303.15	7.4	0.0030	0.001	1.26
303.15	7.4	0.0050	0	1.66
303.15	7.4	0.0050	0.001	1.41
303.15	7.4	0.0070	0	1.76
303.15	7.4	0.0070	0.001	1.53
303.15	7.4	0.0090	0	1.84
303.15	7.4	0.0090	0.001	1.64
303.15	7.4	0.013	0	2.00
303.15	7.4	0.013	0.001	1.92
303.15	7.4	0.017	0	2.19
303.15	7.4	0.017	0.001	2.14

Reference: Airas (2006)[136]
Method: radioactivity
Buffer: Hepes (0.050 mol dm^{-3}) + KOH
pH: 7.4
Cofactor(s): $Mg(acetate)_2$
Evaluation: A

The K' values given here are shown in Fig. 6 of Airas (2006).[136] The numerical values are based on a private communication from Airas (2006).[137]

4.98. Enzyme: phenylalanine-tRNA ligase (EC 6.1.1.20)

ATP(aq) + L-phenylalanine(aq) + $tRNA^{Phe}$(aq) = AMP(aq) + pyrophosphate(aq) + L-phenylalanyl-$tRNA^{Phe}$(aq)

T/K	pH	$c(Mg^{2+})$ / (mol dm^{-3})	c(spermidine) / (mol dm^{-3})	K'
303.15	7.4	0.0010	0	0.87
303.15	7.4	0.0010	0.001	0.96
303.15	7.4	0.0020	0	1.01
303.15	7.4	0.0020	0.001	1.04
303.15	7.4	0.0030	0	1.17
303.15	7.4	0.0030	0.001	1.17
303.15	7.4	0.0060	0	1.41
303.15	7.4	0.0060	0.001	1.38
303.15	7.4	0.010	0	1.74
303.15	7.4	0.010	0.001	1.75
303.15	7.4	0.014	0	2.25
303.15	7.4	0.014	0.001	2.04
303.15	7.4	0.018	0	2.41
303.15	7.4	0.018	0.001	2.49

Reference: Airas (2007)[152]

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Method: radioactivity
Buffer: Hepes (0.050 mol dm^{-3}) + KOH
pH: 7.4
Cofactor(s): $Mg(acetate)_2$
Evaluation: A

4.99. Enzyme: histidine t-RNA ligase (EC 6.1.1.21)

ATP(aq) + L-histidine(aq) + $tRNA^{His}$(aq) = AMP(aq) + pyrophosphate(aq) + L-histidyl-$tRNA^{His}$(aq)

T/K	pH	$c[Mg^{2+}]$ / (mol dm^{-3})	c(spermidine) / (mol dm^{-3})	K'
303.15	7.4	0.000 50	0	1.23
303.15	7.4	0.000 50	0.001	0.93
303.15	7.4	0.0015	0	1.24
303.15	7.4	0.0015	0.001	1.03
303.15	7.4	0.0025	0	1.33
303.15	7.4	0.0025	0.001	1.13
303.15	7.4	0.0035	0	1.43
303.15	7.4	0.0035	0.001	1.35
303.15	7.4	0.0055	0	1.65
303.15	7.4	0.0055	0.001	1.65
303.15	7.4	0.0075	0	1.82
303.15	7.4	0.0075	0.001	1.84
303.15	7.4	0.0095	0	2.00
303.15	7.4	0.0095	0.001	1.96
303.15	7.4	0.0135	0	2.16
303.15	7.4	0.0135	0.001	2.39
303.15	7.4	0.0175	0	2.36
303.15	7.4	0.0175	0.001	2.75

Reference: Airas (2006)[137]
Method: radioactivity
Buffer: Hepes (0.050 mol dm^{-3}) + KOH
pH: 7.4
Cofactor(s): $Mg(acetate)_2$
Evaluation: A

4.100. Enzyme: DNA ligase (ATP) (EC 6.5.1.1)

ATP(aq) + (deoxyribonucleotide)$_n$(aq) + (deoxyribonucleotide)$_m$ = AMP(aq) + pyrophosphate(aq) + (deoxyribonucleotide)$_{m+n}$(aq)

T/K	pH	K'
298.15	7.0	$3.89 \cdot 10^4$

Reference: Dickson *et al.* (2001)[98]
Method: spectrophotometry
Buffer: Tris (0.20 mol dm^{-3}) + HCl
pH: 7.0
Cofactor(s): $MgCl_2$ (0.010 mol dm^{-3})
Evaluation: B

5. List of Substances with Chemical Abstract Service (CAS) Registry Numbers with Cross References to Enzyme Commission Numbers

Substance	CAS registry[4] number[a]	Enzyme Commission numbers
acetaldehyde	75-07-0	4.1.2.4
2-acetamidohept-6-enoic acid	166540-75-6	3.5.1.14
acetate	64-19-7	3.5.1.14, 3.4.21.1
acetone	67-64-1	1.1.1.2
N-acetyl-L-alanine	97-69-8	3.5.1.14
acetyl-coenzyme A	72-89-9	2.3.1.169
N-acetyl-L-cysteine	616-91-1	3.5.1.14
N-acetyl-L-methionine	65-82-7	3.5.1.14
N-acetyl-L-norleucine	15891-49-3	3.5.1.14
N-acetyl-L-phenylalanine	2018-61-3	3.5.1.14
3-acetylpyridine adenine dinucleotide(ox)	86-08-8	1.1.1.37
3-acetylpyridine adenine dinucleotide(red)	153-59-3	1.1.1.37
N-acetyl-L-valine	96-81-1	3.5.1.14
acyl-carrier-protein	77322-37-3	2.3.1.129
adenine	73-24-5	2.4.2.7, 2.4.2.28
adenosine 3′:5′-(cyclic)phosphate	60-92-4	3.1.4.17
adenosine 5′-diphosphate	58-64-0	2.7.1.2, 2.7.1.37, 2.7.1.40, 2.7.1.117, 2.7.3.2, 2.7.3.3, 2.7.7.a, 3.6.1.3
adenosine 5′-diphosphoglucose	102129-65-7	3.1.4.a, 2.7.7.a
adenosine 5′-monophosphate	61-19-8	2.4.2.7, 2.7.9.2, 3.1.4.17, 3.1.4.a, 6.1.1.1, 6.1.1.3, 6.1.1.5, 6.1.1.6, 6.1.1.11, 6.1.1.19, 6.1.1.20, 6.1.1.21, 6.5.1.1

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Substance	CAS registry[4] number[a]	Enzyme Commission numbers
adenosine 5′-triphosphate	56-65-5	2.7.1.2, 2.7.1.37, 2.7.1.40, 2.7.1.117, 2.7.2.a, 2.7.3.2, 2.7.3.3, 2.7.7.4, 2.7.9.2, 3.6.1.3, 6.1.1.1, 6.1.1.3, 6.1.1.5, 6.1.1.6, 6.1.1.11, 6.1.1.19, 6.1.1.20, 6.1.1.21,6.5.1.1
adenylylsulfate	102029-95-8	2.7.7.4
D-alanine	338-69-2	5.1.1.1
L-alanine	56-41-7	2.6.1.37, 3.5.1.14, 5.1.1.1
2-aminobenzoic acid	118-92-3	2.7.2.a
3-aminobenzoic acid	99-05-8	2.7.2.a
4-aminobenzoic acid	150-13-0	2.7.2.a
2-aminobenzoic acid adenylate	88609-72-7	2.7.2.a
3-aminobenzoic acid adenylate	937721-58-9	2.7.2.a
4-aminobenzoic acid adenylate	88609-76-1	2.7.2.a
4-aminobutanoate	56-12-2	2.6.1.19
2-amino-2-deoxyisochorismate	97279-79-3	4.1.3.27
(2-aminoethyl)phosphonate	2041-14-7	2.6.1.37
((2*R*,3*S*4*R*,5*R*) -5-(2-amino-5-formamido-6-oxo-3,6-dihydropyrimidin-4-ylamino)-3,4-dihydroxy-tetrahydrofuran-2-yl)methyl tetrahydrogen triphosphate	27089-32-3	3.5.4.16
2-aminohept-6-enoic acid	10325-17-4	3.5.1.14
7-amino-3-((1-methyl-III-tetrazol-5-yl)-thiomethyl)-cephalosporanic acid	24209-38-9	3.5.1.11
6-aminopenicillanic acid	551-16-6	3.5.1.11
ammonia	7664-41-7	1.4.3.6, 3.5.1.1, 3.5.1.2, 3.5.2.2, 3.5.5.1, 4.1.3.27
amoxicillin	61336-70-7	3.5.1.11
anandamide	94421-68-8	3.5.1.a
anthranilate	118-92-3	4.1.3.27
D-arabinose	10323-20-3	5.3.1.5
D-arabinose 5-phosphate	89927-09-3	5.3.1.13
arachidonic acid	506-32-1	3.5.1.a
D-arginine	74-79-3	2.7.3.3, 6.1.1.19
D-arginyl-transfer ribonucleic acid (arginine)	b	6.1.1.19
D-asparagine	70-47-3	3.5.1.1
D-aspartate	56-84-8	2.1.3.2, 3.5.1.1
D-aspartate 4-semialdehyde	15106-57-7	1.1.1.3
benzoic acid	65-85-0	2.7.2.a, 3.5.5.1
benzoic acid adenylate	56164-09-1	2.7.2.a
benzonitrile	100-47-0	3.5.5.1
benzyl acetate	140-11-4	3.1.1.3
benzyl alcohol	100-51-6	3.1.1.3
benzyl cyanide	140-29-4	3.5.5.1
(±)-*cis*-2-benzyl-1-cyclohexanol	5915-08-2	1.1.1.2
(±)-*trans*-2-benzyl-1-cyclohexanol	5947-19-3	1.1.1.2
2-benzyl-1-cyclohexanone	946-33-8	1.1.1.2
1-butanol	71-36-3	3.1.1.3
(±)-2-butanol	78-92-2	1.1.1.2
2-butanone	78-93-3	1.1.1.2
butyl acetate	123-86-4	3.1.1.3
butyl decanoate	30673-36-0	3.1.1.3
1-butyl oleate	142-77-8	3.1.1.3
N-carbamoyl-L-aspartate	16649-79-9	2.1.3.2
carbamoyl phosphate	590-55-6	2.1.3.2
carbon dioxide	124-38-9	1.1.1.87, 3.5.2.2, 4.1.1.3, 4.1.1.23, 4.1.1.39
carbon monoxide	630-08-0	2.3.1.169
3-carboxy-2-hydroxyadipate	26091-87-2	1.1.1.87
L-carnitine	541-15-1	4.2.1.89
cefamandole	34444-01-4	3.5.1.11
(3β,5α)-cholesta-7,24-diene-3-ol	651-54-7	5.3.3.5
(3β,5α)-cholesta-8,24-diene-3-ol	128-33-6	5.3.3.5

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Substance	CAS registry[4] number[a]	Enzyme Commission numbers
chorismate	617-12-9	4.1.3.27, 5.4.99.6
coenzyme A	85-61-0	2.3.1.169
corrinoid protein	b	2.3.1.169
creatine	57-00-1	2.7.3.2
trans-but-2-enoyl-coenzyme A	102680-35-3	4.2.1.17
cyclobutanol	2919-23-5	1.1.1.2
cyclobutanone	1191-95-3	1.1.1.2
cycloheptanol	502-41-0	1.1.1.2
cycloheptanone	502-42-1	1.1.1.2
cyclohexanol	108-93-0	1.1.1.2
cyclohexanone	108-94-1	1.1.1.2
cyclooctanol	696-71-9	1.1.1.2
cyclooctanone	502-49-8	1.1.1.2
cyclopentanol	98-41-3	1.1.1.2
cyclopentanone	120-92-3	1.1.1.2
L-cysteine	52-90-4	3.5.1.14
1-decanoic acid	334-48-5	3.1.1.3
2-dehydro-3-deoxy-D-arabino- 7-heptanoate 7-phosphate	2627-73-8	4.1.2.15, 4.6.1.3
2-keto-L-gulonate	526-98-7	1.1.1.274
2-dehydropantoate	470-30-4	1.1.1.169
3-dehydroquinate	10534-44-8	4.2.1.10, 4.6.1.3
3-dehydroshikimate	2922-42-1	4.2.1.10
2′-deoxyinosine	890-38-0	2.4.2.1
deoxynucleoside triphosphate	b	2.7.7.7
$(\text{deoxyribonucleotide})_n$	b	6.5.1.1
2-deoxy-D-ribose 5-phosphate	102916-66-5	4.1.2.4
2-deoxy-α-D-ribose 1-phosphate	102783-28-8	2.4.2.1
N^6-(L-1,3-dicarboxypropyl)-L-lysine	997-68-2	1.5.1.7
7,8-dihydrofolate	4033-27-6	1.5.1.3
5,6-dihydrouracil	504-07-4	3.5.2.2
2,3-dihydroxybenzoic acid	303-38-8	2.7.2.a
2,3-dihydroxybenzoic acid adenylate	122408-18-8	2.7.2.a
2,5-diketo-D-gluconate	2595-33-7	1.1.1.274
4-dimethylaminomethylbenzaldehyde	36874-95-0	1.4.3.6
4-dimethylaminomethylbenzylamine	34490-85-2	1.4.3.6
3,3-dimethyl-2-oxobutanoate	815-17-8	2.6.1.42
1,2-dioctanoyl glycerol	104195-35-9	3.1.1.3
1,3-dioctanoyl glycerol	1429-66-9	3.1.1.3
1-dodecanoic acid	143-07-7	3.1.1.3
1-dodecanol	112-53-8	3.1.1.3
1-dodecanoyl glucose ester	27836-64-2	3.1.1.3
dodecyl dodecanoate	13945-76-1	3.1.1.3
D-erythrose	583-50-6	5.3.1.5
D-erythrose 4-phosphate	585-18-2	4.1.2.15
D-erythrulose	496-55-9	5.3.1.5
ethanolamine	141-43-5	3.5.1.a
(2*R*,3*R*)-*erythro*-fluoromalate	74806-82-9	1.1.1.37
(3*R*)-fluorooxalacetate	68995-36-8	1.1.1.37
10-formyltetrahydrofolate	2800-34-2	1.5.1.5
D-fructose	57-48-7	3.2.1.26, 5.3.1.5
D-fructose 1,6-bisphosphate	488-69-7	2.7.1.90, 4.1.2.13
D-fructose 6-phosphate	643-13-0	2.7.1.90, 5.3.1.9, 1.1.1.17
D-glucose	50-99-7	2.7.1.2, 3.1.1.3, 3.2.1.26, 5.3.1.5
D-glucose 6-phosphate	56-73-5	2.4.1.216, 2.7.1.2, 5.3.1.9
α-D-glucose 1-phosphate	59-56-3	2.7.7.a, 3.1.4.a
β-D-glucose 1-phosphate	32972-46-6	2.4.1.216
L-glutamate	56-86-0	2.6.1.19, 2.6.1.42, 2.6.1.52, 3.5.1.2
L-glutamine	56-85-9	3.5.1.2

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Substance	CAS registry[4] number[a]	Enzyme Commission numbers
glutathoine(ox)	27025-41-8	1.6.4.2
glutathoine(red)	70-18-8	1.6.4.2
D-glyceraldehyde	453-17-8	4.1.2.a
D-glyceraldehyde 3-phosphate	591-57-1	4.1.2.4, 4.1.2.13
glycerol	56-81-5	3.1.1.3
glycerone phosphate	57-04-5	4.1.2.13
glyoxylate	298-12-4	4.1.3.1
guanosine 3′ 5′-cyclic phosphate	40732-48-7	3.1.4.35
guanosine 5′-phosphate	85-32-5	3.1.4.35
guanosine 5′-triphosphate	56001-37-7	3.5.4.16
H+	12408-02-5	1.15.1.1
H_2	1333-74-0	1.18.99.1
H_2O	7732-18-5	1.1.3.22, 1.4.3.6, 1.5.1.7, 2.7.9.2, 3.1.1.3, 3.1.3.1, 3.1.4.17, 3.1.4.35, 3.1.4.a, 3.2.1.26, 3.2.2.2, 4.21.1, 3.4.21.62, 3.5.1.1, 3.5.1.2, 3.5.1.11, 3.5.1.14, 3.5.1.a, 3.5.4.16, 3.5.5.1, 3.6.1.1, 3.6.1.a, 3.6.1.3, 4.1.2.15, 4.1.3.27, 4.2.1.10, 4.2.1.17, 4.2.1.89
H_2O_2	7722-84-1	1.1.3.22, 1.4.3.6, 1.15.1.1
(*S*)-(+)-2-heptanol	6033-23-4	1.1.1.2
2-heptanone	110-43-0	1.1.1.2
(±)-2-hexanol	626-93-7	1.1.1.2
2-hexanone	591-78-6	1.1.1.2
L-histidine	71-00-1	6.1.1.21
L-histidyl-transfer ribonucleic acid (histidine)	b	6.1.1.21
L-homoserine	672-15-1	1.1.1.3
hydantoin	461-72-3	3.5.2.2
3-hydroxyanthranilic acid	548-93-6	2.7.2.a
3-hydroxyanthranilic acid adenylate	88609-71-6	2.7.2.a
3-hydroxybenzoic acid	99-06-9	2.7.2.a
4-hydroxybenzoic acid	99-96-7	2.7.2.a
3-hydroxybenzoic acid adenylate	88609-73-8	2.7.2.a
4-hydroxybenzoic acid adenylate	937721-59-0	2.7.2.a
4-hydroxybutanoate	591-81-1	1.2.1.a
D-2-hydroxy-*n*-butanoate	20016-85-7	1.1.1.28
(3*S*)-3-hydroxybutanoyl-coenzyme A	22138-45-0	4.2.1.17
cis-2-hydroxycyclopentanemethanol cyclic phosphate	73424-01-8	3.1.3.1, 3.1.4.a
trans-2-hydroxycyclopentanemethanol cyclic phosphate	73581-87-0	3.1.3.1, 3.1.4.a
cis-2-hydroxycyclopentanemethanol α-phosphate	937721-60-3	3.1.3.1, 3.1.4.a
trans-2-hydroxycyclopentanemethanol α-phosphate	73410-66-9	3.1.3.1, 3.1.4.a
3-hydroxy-4-methylbenzoic acid	586-30-1	2.7.2.a
3-hydroxy-4-methylbenzoic acid adenylate	88609-74-9	2.7.2.a
5-(4-hydroxyphenyl) D-carbamoylate	68780-35-8	3.5.2.2
D-(4-hydroxyphenyl)glycine	22818-40-2	3.5.1.11, 3.5.2.2
5-(4-hydroxy)-phenylhydantoin	2420-17-9	3.5.2.2
(*R*)-3-hydroxytetradecanoyl-[acyl-carrier-protein]	937244-36-5	2.3.1.129
(1*R*,2*S*)-*trans*-2-hydroxytetrahydrofuranmethanol cyclic phosphate	73410-60-3	3.1.3.1, 3.1.4.a
(1*R*,2*S*)-*trans*-2-hydroxytetrahydrofuranmethanol α-phosphate	73423-99-1	3.1.3.1, 3.1.4.a
hypoxanthine	68-94-0	2.4.2.1, 3.2.2.2, 2.4.2.1, 2.4.2.8
indole-3-acetic acid	87-51-4	3.5.5.1
3-indoleacetonitrile	771-51-7	3.5.5.1
inosine	58-63-9	3.2.2.2, 2.4.2.1
inosine 5′-monophosphate	131-99-7	2.4.2.8, 3.6.1.a
inosine 5′-triphosphate	132-06-9	3.6.1.a
isochorismate	22642-82-6	5.4.99.6
isocitrate	320-77-4	4.1.3.1
L-isoleucine	73-32-5	6.1.1.5

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Substance	CAS registry[4] number[a]	Enzyme Commission numbers
L-isoleucyl-transfer ribonucleic acid (isoleucine)	b	6.1.1.5
(*R*)-lactate	10326-41-7	1.1.1.28
L-leucine	61-90-5	2.6.1.42
L-*tert*-leucine	20859-02-3	2.6.1.42
L-lysine	56-87-1	1.5.1.7, 6.1.1.6
L-lysyl-transfer ribonucleic acid (lysine)	b	6.1.1.6
(*S*)-malate	97-67-6	1.1.1.37
D-mandelic acid	611-71-2	3.5.1.11
D-mannitol-1-phosphate	104835-69-0	1.1.1.17
D-mannose	3458-28-4	5.3.1.5
(−)-menthol	2216-51-5	3.1.1.3
(−)-menthyl dodecanoate	57084-14-7	3.1.1.3
L-methionine	63-68-3	3.5.1.14
2-methoxy-3-hydroxypropyl phosphate	73410-62-5	3.1.3.1, 3.1.4.a
5-methoxytrimethylene phosphate	73410-61-4	3.1.3.1, 3.1.4.a
α-methylbenzene acetic acid	1823-91-2	3.5.5.1
3-methylbenzoic acid	99-04-7	2.7.2.a
4-methylbenzoic acid	99-94-5	2.7.2.a
3-methylbenzoic acid adenylate	937721-61-4	2.7.2.a
4-methylbenzoic acid adenylate	149834-08-2	2.7.2.a
α-methylbenzylcyanide	1823-91-2	3.5.5.1
methylcorrinoid protein	b	2.3.1.169
(±)-*cis*-2-methyl-1-cyclohexanol	615-38-3	1.1.1.2
(±)-*trans*-2-methyl-1-cyclohexanol	615-39-4	1.1.1.2
2-methyl-1-cyclohexanone	583-60-8	1.1.1.2
5,10-methylenetetrahydrofolate	3432-99-3	1.5.1.5
2-methyl-3-hydroxypropyl phosphate	73410-64-7	3.1.3.1, 3.1.4.a
5′-methylthioadenosine	2457-80-9	2.4.2.28
5-methylthio-D-ribose 1-phosphate	72843-83-5	2.4.2.28
5-methyltrimethylene phosphate	68755-22-6	3.1.3.1, 3.1.4.a
methyl viologen(ox)	4685-14-7	1.18.99.1
methyl viologen(red)	15591-62-5	1.18.99.1
1-monooctanoyl glycerol	19670-49-6	3.1.1.3
2-monooctanoyl glycerol	4228-48-2	3.1.1.3
myosin light chain	b	2.7.1.117
myosin light chain phosphate	b	2.7.1.117
β-nicotinamide-adenine dinucleotide, oxidized form	53-84-9	1.1.1.17, 1.1.1.28, 1.1.1.37, 1.1.1.87, 1.1.1.133, 1.5.1.7, 1.6.1.1, 5.1.3.13
β-nicotinamide-adenine dinucleotide, reduced form	58-68-4	1.1.1.17, 1.1.1.28, 1.1.1.37, 1.1.1.87, 1.1.1.133, 1.5.1.7, 1.6.1.1, 5.1.3.13
β-nicotinamide-adenine dinucleotide phosphate, oxidized form	53-59-8	1.1.1.2, 1.1.1.3, 1.1.1.65, 1.1.1.274, 1.2.1.a, 1.5.1.3, 1.5.1.5, 1.6.1.1, 1.6.4.2
β-nicotinamide-adenine dinucleotide phosphate, reduced form	2646-71-1	1.1.1.2, 1.1.1.3, 1.1.1.65, 1.1.1.274, 1.2.1.a, 1.5.1.3, 1.5.1.5, 1.6.1.1, 1.6.4.2
β-nicotinamide mononucleotide	1094-61-7	2.4.2.11
nicotinic acid	59-67-6	2.4.2.11
4-nitrophenol	100-02-7	3.4.21.1
4-nitrophenyl acetate	830-03-5	3.4.21.1
(4-nitrophenyl)analide	100-01-6	3.4.21.62
L-norleucine	327-57-1	3.5.1.14
$O_2^-\cdot$	11062-77-4	1.15.1.1
O_2	7782-44-7	1.1.3.22, 1.15.1.1, 1.4.3.6, 4.1.1.39
n-octanoic acid	124-07-2	3.1.1.3
(*S*)-(+)-2-octanol	6169-06-8	1.1.1.2
2-octanone	111-13-7	1.1.1.2
oleic acid	112-80-1	3.1.1.3
orotate	65-86-1	2.4.2.10

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Substance	CAS registry[4] number[a]	Enzyme Commission numbers
orotidine 5′-phosphate	2149-82-8	2.4.2.10, 4.1.1.23
orthophosphate	7664-38-2	2.1.3.2, 2.4.1.216, 2.4.2.1, 2.4.2.28, 2.4.2.3, 2.7.1.90, 2.7.9.2, 2.7.7.a, 3.1.3.1, 3.6.1.1, 3.6.1.3, 4.1.2.15, 4.6.1.3
oxaloacetate	328-42-7	1.1.1.37, 4.1.1.3
2-oxoadipate	3184-35-8	1.1.1.87
2-oxobutanoate	600-18-0	1.1.1.28
4-oxobutanoate	692-29-5	1.2.1.a, 2.6.1.19
2-oxo-3-deoxy-D-gluconate	17510-99-5	4.1.2.a
2-oxoglutarate	328-50-7	1.5.1.7, 2.6.1.19, 2.6.1.42, 2.6.1.52
2-oxoisocaproate	816-66-0	2.6.1.42
2-oxovalerate	1821-02-9	2.6.1.42
palmitic acid	57-10-3	3.5.1.a
palmitoylethanolamide	544-31-0	3.5.1.a
(*R*)-pantoate	1112-33-0	1.1.1.169
(±)-2-pentanol	6032-29-7	1.1.1.2
2-pentanone	107-87-9	1.1.1.2
phenylacetic acid	103-82-2	3.5.5.1
L-phenylalanine	63-91-2	3.5.1.14, 6.1.1.20
L-phenylalanyl-transfer ribonucleic acid (phenylalanine)	b	6.1.1.20
4-phenylbutanoic acid	1821-12-1	3.5.5.1
(±)-1-phenyl-1-butanol	21632-18-8	1.1.1.2
(*R*)-(+)-1-phenyl-1-butanol	22144-60-1	3.1.1.3
1-phenyl-1-butanone	495-40-9	1.1.1.2
(*R*)-(+)-1-phenyl 1-butyl acetate	84194-64-9	3.1.1.3
4-phenylbutyronitrile	2046-18-6	3.5.5.1
5-phenyl D-carbamoylate	82264-50-4	3.5.2.2
(±)-*cis*-2-phenyl-1-cyclohexanol	40960-73-4	1.1.1.2
(±)-*trans*-2-phenyl-1-cyclohexanol	40960-69-8	1.1.1.2
2-phenyl-1-cyclohexanone	1444-65-1	1.1.1.2
(±)-1-phenyl-1-ethanol	13323-81-4	1.1.1.2
(*R*)-(+)-1-phenyl ethanol	1517-69-7	3.1.1.3
1-phenyl-1-ethanone	98-86-2	1.1.1.2
(*R*)-(+)-1-phenyl ethyl acetate	16197-92-5	3.1.1.3
D-phenylglycine	69-91-0	3.5.2.2
(±)-1-phenyl-1-heptanol	614-54-0	1.1.1.2
1-phenyl-1-heptanone	1671-75-6	1.1.1.2
(±)-1-phenyl-1-hexanol	4471-05-0	1.1.1.2
1-phenyl-1-hexanone	942-92-7	1.1.1.2
5-phenylhydantoin	27534-86-7	3.5.2.2
(±)-1-phenyl-1-pentanol	21632-19-9	1.1.1.2
1-phenyl-1-pentanone	1009-14-9	1.1.1.2
3-phenylpropanoic acid	501-52-0	3.5.5.1
(±)-1-phenyl-1-propanol	613-86-5	1.1.1.2
(*R*)-(+)-1-phenyl-1-propanol	1565-74-8	3.1.1.3
1-phenyl-1-propanone	93-55-0	1.1.1.2
3-phenylpropionitrile	645-59-0	3.5.5.1
(*R*)-(+)-1-phenyl-1-propyl acetate	84275-44-5	3.1.1.3
N^{ω}-phospho-L-arginine	1189-11-3	2.7.3.3
phosphocreatine	6190-45-0	2.7.3.2
2-phospho-D-glycerate	70195-25-4	5.4.2.1
3-phopho-D-glycerate	80731-10-8	4.1.1.39, 5.4.2.1
2-phosphonoacetaldehyde	16051-76-6	2.6.1.37
3-phosphonooxypyruvate	3913-50-6	2.6.1.52
3-phosphonopyruvate	5824-58-8	5.4.2.9
phospho*enol*pyruvate	138-08-9	2.7.1.40, 2.7.9.2, 3.1.3.1, 4.1.2.15, 5.4.2.9
5-phospho-α-D-ribose 1-diphosphate	108321-05-7	2.4.2.7, 2.4.2.8, 2.4.2.10, 2.4.2.11
phosphorylated serpeptide	78844-90-3	2.7.1.37

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Substance	CAS registry[4] number[a]	Enzyme Commission numbers
O-phospho-L-serine	407-41-0	2.6.1.52
phosphosyntide	357062-25-0	2.7.1.37
poly(deoxyadenylic-thymidilic) acid	86828-69-5	2.7.7.7
2-propanol	67-63-0	1.1.1.2
pyridoxal	66-72-8	1.1.1.65
pyridoxine	65-23-6	1.1.1.65
pyrophosphate	2466-09-3	2.4.2.7, 2.4.2.8,2.4.2.10, 2.4.2.11, 2.7.1.90, 2.7.2.a, 3.6.1.1, 3.6.1.a, 2.7.7.4, 2.7.7.7, 6.1.1.1, 6.1.1.3, 6.1.1.5, 6.1.1.6, 6.1.1.11, 6.1.1.19, 6.1.1.20, 6.1.1.21, 6.5.1.1
pyruvate	127-17-3	1.1.1.28, 2.6.1.37, 2.7.1.40, 2.7.9.2, 3.1.3.1, 4.1.1.3, 4.1.2.a, 4.1.3.27
D-ribose	50-69-1	3.2.2.2, 5.3.1.5
α-D-ribose 1-phosphate	18646-11-2	2.4.2.1, 2.4.2.3
D-ribulose	488-84-6	5.3.1.5
D-ribulose 1,5-bisphosphate	24218-00-6	4.1.1.39
D-ribulose 5-phosphate	551-85-9	5.3.1.13
L-serine	56-45-1	6.1.1.11
serpeptide (Leu-Arg-Arg-Ala-Ser-Leu-Gly)	65189-71-1	2.7.1.37
L-seryl-transfer ribonucleic acid (serine)	b	6.1.1.11
succinate	110-15-6	4.1.3.1
succinylAla-Ala-Pro-Leu	937721-62-5	3.4.21.62
succinylAla-Ala-Pro-Leu-(4-nitrophenyl)analide	70968-04-6	3.4.21.62
succinylAla-Ala-Pro-Phe	108693-50-1	3.4.21.62
succinylAla-Ala-Pro-Phe-(4-nitrophenyl)analide	70967-97-4	3.4.21.62
sucrose	57-50-1	3.2.1.26
sulfate	7664-93-9	2.7.7.4
syntide 2 (Pro-Leu-Ala-Arg-Thr-Leu-Ser-Val-Ala-Gly-Leu-Pro-Gly-Lys-Lys)	108334-68-5	2.7.1.37
5,6,7,8-tetrahydrofolate	135-16-0	1.5.1.3
L-threonine	72-19-5	6.1.1.3
L-threonyl-transfer ribonucleic acid (threonine)	b	6.1.1.3
D-threose	95-43-2	5.3.1.5
thymidine 5′-diphospho-6-deoxy-L-lyxo-4-hexulose	16760-43-3	1.1.1.133
thymidine 5′-diphospho-6-deoxy-D-xylo-4-hexulose	16752-71-9	1.1.1.133, 5.1.3.13
thymidine 5′-diphospho-L-rhamnose	2147-59-3	1.1.1.133, 5.1.3.13
α,α-trehalose 6-phosphate	136632-28-5	2.4.1.216
transfer ribonucleic acid (arginine)	b	6.1.1.19
transfer ribonucleic acid (histidine)	b	6.1.1.21
transfer ribonucleic acid (isoleucine)	b	6.1.1.5
transfer ribonucleic acid (lysine)	b	6.1.1.6
transfer ribonucleic acid (phenylalanine)	b	6.1.1.20
transfer ribonucleic acid (serine)	b	6.1.1.11
transfer ribonucleic acid (threonine)	b	6.1.1.3
transfer ribonucleic acid (tyrosine)	b	6.1.1.1
4-(trimethylammonio)but-2-enoate	927-89-9	4.2.1.89
1,2,3-trioctanoyl glycerol	538-23-8	3.1.1.3
L-tyrosine	60-18-4	6.1.1.1
L-tyrosyl-transfer ribonucleic acid (tyrosine)	b	6.1.1.1
uracil	66-22-8	2.4.2.3
urate	69-93-2	1.1.3.22
ureidoacetic acid	462-60-2	3.5.2.2
3-ureidopropanoic acid	462-88-4	3.5.2.2
uridine	58-96-8	2.4.2.3
uridine 5′-diphospho-*N*-acetyl-D-galactosamine	2616-63-9	5.1.3.2
uridine 5′-diphospho-*N*-acetyl-D-glucosamine	91183-98-1	2.3.1.129, 5.1.3.2
uridine 5′-diphosphogalactose	89705-69-1	5.1.3.2

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Substance	CAS registry[4] number[a]	Enzyme Commission numbers
uridine 5′-diphospho-D-galacturonate	148407-07-2	5.1.3.6
uridine 5′-diphosphoglucose	133-89-1	5.1.3.2
uridine 5′-diphospho-D-glucuronate	7305-43-3	5.1.3.6
uridine 5′-diphospho-3-*O*-(3-hydroxytetradecanoyl)-*N*-acetyl-D-glucosamine	937721-63-6	2.3.1.129
uridine 5′-monophosphate	58-97-9	4.1.1.23
L-valine	72-18-4	2.6.1.42, 3.5.1.14
xanthine	69-89-6	1.1.3.22

[a] In some cases, the CAS registry number refers to a salt of the substance.
[b] In the absence of a sequence, no CAS registry number is assigned to this substance.

6. Abbreviations

acetyl-CoA	acetyl-coenzyme A
ADP	adenosine 5′-diphosphate
ADPglucose	adenosine 5′-diphosphoglucose
AMP	adenosine 5′-monophosphate
L-arginyl-tRNA^{Arg}	L-arginyl-transfer ribonucleic acid (arginine)
ATP	adenosine 5′-triphosphate
Bes	*N*,*N*-bis[2-hydroxyethyl]-2-aminoethanesulfonic acid
Bis-Tris	bis(2-hydroxyethyl)iminotris(hydroxymethyl)methane
Bis-tris propane	1,3-bis[tris(hydroxymethyl)methylamino]propane
Ches	2-(cyclohexylamino)ethanesulfonic acid
CoA	coenzyme A
dTDP-6-deoxy-L-xylo-4-hexulose	thymidine-5′-diphospho-6-deoxy-L-xylo-4-hexulose
dTDP-L-rhamnose	thymidine-5′-diphospho-L-rhamnose
GTP	guanosine 5′-triphosphate
Hepes	*N*-(2-hydroxyethyl)piperazine-*N*′-2-ethanesulfonic acid
L-histidyl-tRNA^{His}	L-histidyl-transfer ribonucleic acid (histidine)
IMP	inosine 5′-monophosphate
L-isoleucyl-tRNA^{Ile}	L-isoleucyl-transfer ribonucleic acid (isoleucine)
ITP	inosine 5′-triphosphate
L-lysyl-tRNA^{lys}	L-lysyl-transfer ribonucleic acid (lysine)
Mes	2-[*N*-morpholino]ethanesulfonic acid
Mops	3-(*N*-morpholino)propanesulfonic acid
NAD(ox)	β-nicotinamide-adenine dinucleotide, oxidized form
NAD(red)	β-nicotinamide-adenine dinucleotide, reduced form
NADP(ox)	β-nicotinamide-adenine dinucleotide phosphate, oxidized form
NADP(red)	β-nicotinamide-adenine dinucleotide phosphate, reduced form
L-phenylalanyl-tRNA^{Phe}	L-phenylalanyl-transfer ribonucleic acid (phenylalanine)
Pipes	piperazine-*N*,*N*′-bis(2-ethanesulfonic acid)
poly[d-(A-T)]$_n$	poly(deoxyadenylic-thymidilic) acid
L-seryl-tRNA^{Ser}	L-seryl-transfer ribonucleic acid (serine)
Tes	*N*-tris(hydroxymethyl)methyl-2-aminoethanesulfonic acid
L-threonyl-tRNA^{Thr}	L-threonyl-transfer ribonucleic acid (threonine)
Tricine	*N*-tris(hydroxymethyl)methylglycine
Tris	2-amino-2-hydroxymethylpropane-1,3 diol
tRNA^{Arg}	transfer ribonucleic acid (arginine)
tRNA^{His}	transfer ribonucleic acid (histidine)
tRNA^{Ile}	transfer ribonucleic acid (isoleucine)
tRNA^{Lys}	transfer ribonucleic acid (lysine)
tRNA^{Phe}	transfer ribonucleic acid (phenylalanine)
tRNA^{Ser}	transfer ribonucleic acid (serine)
tRNA^{Thr}	transfer ribonucleic acid (threonine)
tRNA^{Tyr}	transfer ribonucleic acid (tyrosine)
L-tyrosyl-tRNA^{Tyr}	L-tyrosyl-transfer ribonucleic acid (tyrosine)
UDP-*N*-acetyl-D-galactosamine	uridine-5′-diphospho-*N*-acetyl-D-galactosamine
UDP-*N*-acetyl-D-glucosamine	uridine-5′-diphospho-*N*-acetyl-D-glucosamine

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UDPgalactose	uridine 5′-diphosphogalactose
UDP-D-galacturonate	uridine-5′-diphospho-D-galacturonate
UDPglucose	uridine-5′-diphosphoglucose
UDP-D-glucuronate	uridine-5′-diphosphoglucuronate
UDP-3-*O*-(3-hydroxytetradecanoyl)-*N*-acetylglucosamine	uridine-5′-diphospho-3-*O*-(3-hydroxytetradecanoyl)-*N*-acetylglucosamine
UMP	uridine 5′-monophosphate

7. Glossary of Symbols

Symbol	Name	Unit
c	concentration	mol dm^{-3}
c°	standard concentration ($c^\circ = 1$ mol dm^{-3})	mol dm^{-3}
$\Delta_r C_P^\circ$	standard molar heat capacity of reaction at constant pressure	J K^{-1} mol^{-1}
$\Delta_r G^\circ$	standard molar Gibbs energy of reaction	kJ mol^{-1}
$\Delta_r G'^\circ$	standard molar transformed Gibbs energy of reaction	kJ mol^{-1}
$\Delta_r H^\circ$	standard molar enthalpy of reaction	kJ mol^{-1}
$\Delta_r H'^\circ$	standard molar transformed enthalpy of reaction	kJ mol^{-1}
$\Delta_r H$(cal)	calorimetrically determined molar enthalpy of reaction	kJ mol^{-1}
I_c	ionic strength, concentration basis	mol dm^{-3}
I_m	ionic strength, molality basis	mol kg^{-1}
K	equilibrium constant[a]	dimensionless
K'	apparent equilibrium constant[a]	dimensionless
m	molality	mol kg^{-1}
m°	standard molality ($m^\circ = 1$ mol kg^{-1})	mol kg^{-1}
$\Delta_r N(H^+)$	change in binding of hydrogen ion in a biochemical reaction	dimensionless
P	pressure	Pa
pH	$-\log_{10}[c(H^+)/c^\circ]$[b]	dimensionless
pX	$-\log_{10}[c(X)/c^\circ]$	dimensionless
$\Delta_r S^\circ$	standard molar entropy of reaction	J K^{-1} mol^{-1}
T	thermodynamic temperature	K
x	mole fraction	dimensionless

[a] When needed, a subscript c, m, or x is added to these quantities to designate a concentration, molality, or mole fraction basis.
[b] This is an approximate definition. The IUPAC Green Book [I. Mills, T. Cvitaš, K. Homann, N. Kallay, and K. Kuchitsu, *Quantities, Units and Symbols in Physical Chemistry* (Blackwell Scientific, Oxford, 1993)] contains a discussion of the operational definition of pH.

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