Journal of Medicinal Chemistry

Standard Abbreviations and Acronyms

α	observed optical rotation in degrees
[α]	specific rotation [expressed without units; the units, (deg·mL)/(g·dm), are understood]
δ	chemical shift in parts per million downfield from tetramethylsilane
μ	micro
Å	angstrom(s)
°C	degrees Celsius
2-D	two-dimensional (also 2D)
3-D	three-dimensional (also 3D)
5HT	5-hydroxytryptamine (serotonin)
9-BBN	9-borabicyclo[3.3.1]nonyl
9-BBN–H	9-borabicyclo[3.3.1]nonane
Aβ	amyloid β-protein
aa	amino acid
AA	arachidonic acid
Ac	acetyl
Acac	acetylacetonate
AcCh; ACh	acetylcholine
AcChE; AChE	acetylcholine esterase
ACE	angiotensin-converting enzyme
ACP	acyl carrier protein
ACTH	adrenocorticotropic hormone
AD	Alzheimer's disease
ADH	antidiuretic hormone
ADME	absorption, distribution, metabolism and excretion
ADMET	absorption, distribution, metabolism, excretion, and toxicity
ADP	adenosine 5'-diphosphate
ADR	adverse drug reaction
AE	adverse event
AIBN	2,2'-azobisisobutyronitrile
AIDS	acquired immune deficiency syndrome
ALK	anaplastic lymphoma kinase
ALS	amyotrophic lateral sclerosis
AM1	Austin model 1
AMI	acute myocardial infarction
AML	acute myelogenous leukemia
AMP	adenosine 5'-monophosphate; adenosine 5'-phosphate
AMPA	2-amino-3-(3-hydroxy-5-methyl-4-isoxazolyl)propionic acid
Anal.	combustion elemental analysis
anhyd; anh	anhydrous
ANP	atrial natriuretic peptide
antilog	antilogarithm
AO	atomic orbital
API	active pharmaceutical ingredient
ApoB	Apolipoprotein B
ApoE	Apolipoprotein E
APP	amyloid-β precursor protein
aq	aqueous
Ar	aryl
ARB	angiotensin receptor blocker
ARDS	adult respiratory distress syndrome
atm	atmosphere(s)
ASO	antisense oligonucleotide
ATP	adenosine 5'-triphosphate
ATPase	adenosine triphosphatase
AUC	area under the curve
b.i.d.	twice a day
B3LYP	3-parameter hybrid Becke exchange/Lee–Yang–Parr correlation functional
BACE	beta-site amyloid precursor protein cleaving enzyme
BACE-1	beta-secretase
BBB	blood-brain barrier
BChE; BuChE	butyrylcholinesterase
Bcl-xL	B-cell lymphoma-extra large
BMI	body mass index
Bn	benzyl
BOC, boc	*tert*-butoxycarbonyl
bp	boiling point; base pair
BPH	Benign Prostatic Hypertrophy
BRCA1	breast cancer gene 1
BSA	bovine serum albumin
Bu, *n*-Bu	normal (primary) butyl
BUN	blood urea nitrogen
Bz	benzoyl (not benzyl)
ca.	circa, about [used before an approximate date or figure (ca. 1960)]
CADD	computer-assisted drug design
calcd	calculated
cAMP	3',5'-cyclic adenosine monophosphate
CAN	ceric ammonium nitrate
CASPT2	complete active space with second-order perturbation theory
CASSCF	complete active space self-consistent field
cat	catalytic
CB	cannabinoid
CBC	complete blood count
CBZ, Cbz	benzyloxycarbonyl (preferred over the abbreviation Z)
CC	coupled cluster
CCK	cholecystokinin
CD	circular dichroism
CDC	center for disease control

CDER	Center for Drug Evaluation and Research, FDA
CDK	cyclin-dependent kinase
cDNA	complementary deoxyribonucleic acid
CETP	cholesteryl ester transfer protein
cGLP	current good laboratory practices
cGMP	current good manufacturing practice; 3,5'-cyclic guanosine monophosphate
CGRP	calcitonin gene-related peptide
CHF	congestive heart failure
CHK1	checkpoint kinase 1
CHK2	checkpoint kinase 2
CHMP	Committee for Medicinal Products for Human Use
Ci	curie
CI	chemical ionization; configuration interaction
CIDNP	chemically induced dynamic nuclear polarization
CIF	crystallographic information file
CKD	chronic kidney disease
cLopP	calculated logP
cm	centimeter(s)
cm^{-1}	wavenumber(s)
CML	chronic myelogenous leukemia
CMV	cytomegalovirus
CNS	central nervous system
CoA	coenzyme A
cod	1,5-cyclooctadiene
CoMFA	comparative molecular field analysis
compd	compound
CoMSIA	computational molecular similarity index analysis
concd	concentrated
conc; concn	concentration
COPD	chronic obstructive pulmonary disease
CoQ	coenzyme Q10
COSY	correlation spectroscopy
COX	cyclooxygenase
Cp	cyclopentadienyl
CRH	corticotrophin-releasing hormone
CRP	C-reactive protein
CSF	cerebrospinal fluid
CV	cyclic voltammetry
Cy	cyclohexyl
CYP	cytochrome P
d	day(s); doublet (spectral); deci
d	density
DA	dopamine
DABCO	1,4-diazabicyclo[2.2.2]octane
DART	developmental and reproductive toxicology
DAT	dopamine transporter
DBN	1,5-diazabicyclo[4.3.0]non-5-ene
DBP	diastolic blood pressure
DBU	1,8-diazabicyclo[5.4.0]undec-7-ene
DCC	*N,N'*-dicyclohexylcarbodiimide
DCE	1,2-dichloroethane
DCM	dichloromethane
DDI	drug-drug interaction
DDQ	2,3-dichloro-5,6-dicyano-1,4-benzoquinone
DDT	1,1,1-trichloro-2,2-bis(p-chlorophenyl)ethane
de	diastereomeric excess
DEAD	diethyl azodicarboxylate
dec	decomposition
DEPT	distortionless enhancement by polarization transfer
DFT	density functional theory
DIBALH	diisobutylaluminum hydride
DIO	diet induced obesity
DLT	dose limiting toxicity
DMA	dimethylacetamide
DMAP	4-(*N,N*-dimethylamino)pyridine
DMDO	dimethyldioxirane
DME	1,2-dimethoxyethane
DMF	dimethylformamide
DMPK	drug metabolism and pharmacokinetics
DMPU	1,3-dimethyl-3,4,5,6-tetrahydro-2(1*H*)-pyrimidinone
DMSO	dimethyl sulfoxide
DMT	4,4'-dimethoxytrityl (4,4'-dimethoxyltriphenylmethyl)
DNA	deoxyribonucleic acid
Dopa	3-(3,4-dihydroxyphenyl)alanine (also DOPA)
DTT	dithiothreitol
e.g.	for example (exempli gratia)
E1	unimolecular elimination
E2	bimolecular elimination
EC_{50}	half maximal effective concentration
ECG	electrocardiogram
ED_{50}	dose effective in 50% of test subjects
EDTA	ethylenediaminetetraacetic acid
ee	enantiomeric excess
EEG	electroencephalogram
EGF	epidermal growth factor
EGFR	epidermal growth factor receptor
EI	electron impact
EKG	electrocardiogram
ELISA	enzyme-linked immunosorbent assay
EPR	electron paramagnetic resonance
eq	equation
equiv	equivalent
er	enantiomer ratio
ERK	extracellular regulated kinase
ESI	electrospray ionization
ESR	electron spin resonance
Et	ethyl
et al.	and others
etc.	and so forth
F%	% oral bioavailability
FAAH	fatty acid amide hydrolase
FAB	fast atom bombardment

FAD	flavin adenine dinuleotide
FaSSIF	fasted state simulated intestinal fluid
FBDD	fragment-based drug discovery
FD	field desorption
FDA	Food and Drug Administration
FeSSIF	fed state simulated intestinal fluid
FGF	fibroblast growth factor
FID	flame ionization detector; free induction decay
Fmoc	9-fluorenylmethoxycarbonyl
FRET	Förster resonance energy transfer
FSH	follicle-stimulating hormone
FT	Fourier transform
g	gram(s); prefix to NMR abbreviation denoting gradient-selected (e.g. gCOSY, gHMQC)
GABA	γ-aminobutyric acid
GC	gas chromatography
GDP	guanosine 5'-diphosphate
GERD	gastroesophogeal reflux disease
GFP	green fluorescent protein
GFR	glomerular filtration rate
GI	gastrointestinal
GLP-1	glucagon like peptide-1
GlyR	glycine receptor
GMP	guanosine 5'-monophosphate; guanosine 5'-phosphate
GnRH	gonadotropin-releasing hormone
GPCR	G-protein coupled receptor
GFR	growth factor receptor
GST	glutathione S-transferase
GTP	guanosine 5'-triphosphate
h	hour(s); human
HBA	hydrogen bond acceptors
HBD	hydrogen bond donors
HBV	hepatitis B virus
HCS	high-content screening
HCV	hepatitis C virus
HDAC	histone deacetylase
hERG	human Ether-a-go-go-Related Gene
HDL-C	high-density lipoprotein cholesterol
HEK	human embryonic kidney
HF	Hartree–Fock
HGH	human growth hormone
HIV	human immunodeficiency virus
HMBC	heteronuclear multiple bond correlation
HMPA	hexamethylphosphoric triamide (hexamethylphosphoramide)
HMQC	heteronuclear multiple quantum correlation
HOMO	highest occupied molecular orbital
HPLC	high-performance liquid chromatography; high-pressure liquid chromatography
HPV	human papilloma virus
HR	heart rate
HRMS	high-resolution mass spectrometry
HRT	hormone replacement therapy
HSA	human serum albumin
HSP	heat shock protein
HSQC	heteronuclear single quantum correlation
HSV	herpes simplex virus
HTS	high throughput screening
Hz	hertz
i-NOS	inducible nitric oxide synthase
i-Pr	isopropyl
IC_{50}	half-maximum inhibitory concentration
IBD	inflammatory bowel disease
IBS	irritable bowel syndrome
ICR	ion cyclotron resonance
icv	intracerebroventricular (dosing)
Ig	immunoglobulin
iGluR	ionotropic glutamate receptor
IHC	immunohistochemistry
IM	intramuscularly
INDO	intermediate neglect of differential overlap
ip	intraperitoneally
IP	ionization potential
IR	infrared
it	intrathecal
iv	intravenous
IVUS	intravascular ultrasound
J	coupling constant (in NMR spectrometry)
K	kelvin(s) (absolute temperature)
k	kilo
K_i	inhibition constant
Km	Michaelis constant
L	liter(s)
LAH	lithium aluminum hydride
LBD	ligand binding domain
LC	liquid chromatography
LC-MS	liquid chromatography-mass spectrometry
LCAO	linear combination of atomic orbitals
LD_{50}	dose that is lethal in 50% of test subjects
LDA	lithium diisopropylamide; local density approximation
LDL-C	low-density lipoprotein cholesterol
LE	ligand efficiency
LFER	linear free energy relationship
LFT	liver function test
LH	luteinizing hormone
LHMDS	lithium hexamethyldisilazane; lithium bis(trimethylsilyl)amide
LHRH	luteinizing hormone releasing hormone
lit.	literature value (abbreviation used with period)
LogP	logarithm of partition coefficient
LPS	lipopolysaccharide

LTMP	lithium 2,2,6,6-tetramethylpiperidide
LTP	long-term potentiation
LUMO	lowest unoccupied molecular orbital
M	molar (moles per liter); mega
m	multiplet (spectral); meter(s); milli; isotopic mass; magnetic quantum number (ESR and NMR spectroscopy); meta; molal (mol kg-1)
m-CPBA	*meta*-chloroperoxybenzoic acid
m/z	mass-to-charge ratio (not *m/e*)
M^+	parent molecular ion
mAcChR	muscarinic ACh receptor
MALDI	matrix-assisted laser desorption ionization
MAP	mean arterial pressure
MAPK	mitogen-activated protein kinase
max	maximum
MCD	magnetic circular dichroism
MCR	multicomponent reaction
MCSCF	multi-configuration self-consistent field
MD	molecular dynamics
MDR	multidrug resistance
Me	methyl
MED	medium effective dose/minimum efficacious dose
MEM	(2-methoxyethoxy)methyl
Mes	2,4,6-trimethylphenyl (mesityl) [not methylsulfonyl (mesyl)]
mGluR	metabotropic glutamate receptor
MHC	major histocompatibility complex
MHz	megahertz
MIC	minimal inhibitory concentration
min	minute(s); minimum
mL	milliliter
mM	millimolar (millimoles per liter)
MMP	matrix metalloproteinase
MO	molecular orbital
MOA	mechanism of action
mol	mole(s); molecular (as in mol wt)
MOM	methoxymethyl
mp	melting point
MP	Møller–Plesset perturbation theory
MRCI	multi-reference configuration interaction
MRSA	methicillin-resistant Staphylococcus aureus
MRI	magnetic resonance imaging
mRNA	messenger RNA
mRNA	messenger ribonucleic acid
MRSA	methicillin-resistant Staphylococcus aureus
MS	mass spectrometry
Ms	methylsulfonyl (mesyl)
MTBE	methyl *tert*-butyl ether
MTD	maximum tolerated dose
MW, mol wt	molecular weight
nAcChR	nicotinic ACh receptor
NAD^+	nicotinamide adenine dinucleotide
NADH	reduced nicotinamide adenine dinucleotide
NADP	nicotinamide adenine dinucleotide phosphate
NADPH	reduced nicotinamide adenine dinucleotide phosphate
NAM	negative allosteric modulator
NBO	natural bond orbital
NBS	*N*-bromosuccinimide
NCE	new chemical entity
NCI	National Cancer Institute
NCS	*N*-chlorosuccinimide
NDA	new drug application
NE	norepinephrine
NF-kB	nuclear factor k B
NICS	nucleus-independent chemical shift
NIH	National Institutes of Health
nm	nanometer(s)
NMDA	*N*-methyl-D-aspartic acid
NME	new molecular entity
NMO	*N*-methylmorpholine-*N*-oxide
NMP	*N*-methylpyrrolidone
NMR	nuclear magnetic resonance
NNRTI	non-nucleoside reverse transcriptase inhibitor
NO	nitric oxide
NOAEL	no adverse effect level
NOE	nuclear Overhauser effect
NOEL	no-effect level
NOESY	nuclear Overhauser effect spectroscopy
NOS	nitric oxide synthase
NPY	neuropeptide Y
NRT	natural resonance theory
NRTI	nucleoside reverse transcriptase inhibitor
NSAID	non-steroidal anti-inflammatory drug
NSCLC	non-small cell lung cancer
Nu	nucleophile
o	ortho
obsd	observed
OCT	organic cation transporter
OD	optical density
ORD	optical rotary dispersion
p	para
PAF	platelet activating factor
PAGE	polyacrylamide gel electrophoresis
PAM	positive allosteric modulator
PAMPA	parallel artificial membrane permeability assay
PAS	peripheral anionic site
PBO	placebo
PBS	phosphate buffered saline
PCA	principle component analysis
PCC	pyridinium chlorochromate
PCR	polymerase chain reaction
PD	pharmacodynamics; Parkinson's disease

PDB	Protein Data Bank
PDC	pyridinium dichromate
PDE	phosphodiesterase
PEG	polyethylene glycol
PES	photoelectron spectroscopy
PET	positron emission tomography
P-gp	P-glycoprotein
Ph	phenyl
PI3K	phosphoinositide 3-kinase
PIPES	1,4-piperazinediethanesulfonic acid; piperazine-N,N'-bis(2-ethanesulfonic acid)
PK	pharmacokinetics
PKA	protein kinase A
PKB	protein kinase B
PKC	protein kinase C
PLS	partial least squares
pm	picometer(s)
PM3	parametric method 3
PMB	*p*-methoxybenzyl
PNS	peripheral nervous system
po	oral administration
PPA	poly(phosphoric acid)
PPAR	peroxisome proliferator-activated receptor
PPB	plasma protein binding
ppm	part(s) per million
PPTS	pyridinium *para*-toluenesulfonate
Pr	propyl
PRH	prolactin releasing hormone
PSA	polar surface area
psi	pounds per square inch
PT	perturbation theory; prothrombin time
PTT	partial thromboplastin time
PTC	phase-transfer catalysis
PTH	parathyroid hormone
PXR	pregnane X receptor
py	pyridine
q	quartet (spectral)
q.d.	once daily ("quaque die")
q.i.d.	four times a day (dosing) ("quater in die")
QSAR	quantitative structure–activity relationship
QSPR	quantitative structure-property relationship
QW	once a week (dosing)
RAS	renin-angiotensin system
RBC	red blood cell
RCM	ring-closure metathesis
redox	reduction–oxidation
R_f	retention factor (in chromatography)
RHF	restricted Hartree–Fock
RIA	radioimmunoassay
rmsd	root mean square deviation
RNA	ribonucleic acid
RO5	rule of five (Lipinski)
ROESY	rotating frame Overhauser effect spectroscopy
ROMP	ring-opening metathesis polymerization
ROS	reactive oxygen species
rpm	revolutions per minute
rRNA	ribosomal ribonucleic acid
rt	room temperature
s	singlet (spectral); second(s)
s-Bu	*sec*-butyl
SAHA	suberoylanilide hydroxamic acid
SAR	structure–activity relationship
SARM	selective androgen receptor modulator
SBDD	structure-based drug discovery
SBP	systolic blood pressure
sc	subcutaneous
SCF	self-consistent field
SDS	sodium dodecyl sulfate
SEM	scanning electron microscopy
SERM	selective estrogen-receptor modulator
SERT	serotonin transporter
SET	single electron transfer
SFC	supercritical fluid chromatography
SIRT1	silent mating type information regulation 2 homolog 1
S_N'	nucleophilic substitution with allylic rearrangement
S_N1	unimolecular nucleophilic substitution
S_N2	bimolecular nucleophilic substitution
SNP	single nucleotide polymorphism
SOMO	single-occupied molecular orbital
SPECT	single-photon emission computed tomography
PR	surface plasmon resonance; stroboscopic pulse radiolysis
SSRI	selective serotonin reuptake inhibitor
T	absolute temperature in units of kelvins (K)
t	time; temperature in units of degrees Celsius (ºC)
t	triplet (spectral)
t-Bu	*tert*-butyl
$t_{1/2}$	half-time
t.i.d.	three times daily ("ter in die")
T2DM	type 2 diabetes mellitus
TAE	tris-acetate-EDTA
TB	tuberculosis
TBAB	tetrabutylammonium bromide
TBAC	tetrabutylammonium chloride
TBAF	tetrabutylammonium fluoride
TBHP	*tert*-butyl hydroperoxide
TBS	*tert*-butyldimethylsilyl
TCA	trichloroacetic acid
TCA	tricyclic antidepressant
TCNE	tetracyanoethylene
TDDFT	time-dependent density functional theory
TEAB	tetraethylammonium bromide
temp	temperature

Tf	trifluoromethanesulfonyl (triflyl)
TFA	trifluoroacetic acid
TFAA	trifluoroacetic anhydride
THF	tetrahydrofuran
THP	tetrahydropyran-2-yl
TIPS	triisopropylsilyl
TK	toxicokinetics
TLC	thin-layer chromatography
TLR	toll-like receptor
TMAI	tetramethylammonium iodide
TMEDA	*N,N,N′,N′*-tetramethyl-1,2-ethylenediamine
TMS	trimethylsilyl; tetramethylsilane
TNF	tumor necrosis factor
TNF-alpha	tumor necrosis factor-alpha
TOF	time of flight
TON	turn over number (in catalysis)
^{t}R	retention time (in chromatography)
Tr	triphenylmethyl (trityl)
Tris	tris(hydroxymethyl)aminomethane
tRNA	transfer ribonucleic acid
Ts	para-toluenesulfonyl (tosyl)
TS	transition state
TSH	thyroid stimulating hormone
TT	thrombin time
UDP	uridine 5'-diphosphate
UHF	unrestricted Hartree–Fock
UHPLC	ultra-high pressure liquid chromatography
UV	ultraviolet
v.i.	see below (vide infra)
v.s.	see above (vide supra)
v/v	volume per unit volume (volume-to-volume ratio)
VCD	vibrational circular dichroism
VEGFR	vascular endothelial growth factor receptor
vis	visible
viz.	namely
VLDL	very low density lipoprotein
vol	volume
VRE	vancomycin resistant enterococci
WBA	whole body autoradiography
w/w	weight per unit weight (weight-to-weight ratio)
WT	wild type
wt	weight
XAFS	X-ray absorption fine structure spectroscopy
ZINDO	Zerner parameterization of intermediate neglect of differential overlap

STANDARD AMINO ACID ABBREVIATIONS:

•The three-letter code or name may be used in the text.

•With a single amino acid, use the three-letter code (e.g., Met246).

•If more than one amino acid is specified, as in mutants or substitutions, use one-letter code (S238H).

•When two or more amino acids are used in a string, use either the three-letter code or single letter (e.g., His-Ile-Thr-Ser or HITS).

•For use of D amino acids, use the 3 letter abbreviation only (e.g., DAla)

alanine	Ala	A	leucine	Leu	L
arginine	Arg	R	lysine	Lys	K
asparagine	Asn	N	methionine	Met	M
aspartic acid	Asp	D	phenylalanine	Phe	F
cysteine	Cys	C	proline	Pro	P
glutamic acid	Glu	E	serine	Ser	S
glutamine	Gln	Q	threonine	Thr	T
glycine	Gly	G	tryptophan	Trp	W
histidine	His	H	tyrosine	Tyr	Y
isoleucine	Ile	I	valine	Val	V

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