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### List of Abbreviations

<b>Abbreviation</b>	<b>Full Form</b>
<b>2D</b>	Two-dimensional
<b>3D</b>	Three-dimensional
<b>A549</b>	Human lung adenocarcinoma cell line
<b>ACN</b>	Acetonitrile
<b>ADMET</b>	Absorption, Distribution, Metabolism, Excretion & Toxicity
<b>Akt</b>	Protein kinase B
<b>ALOX5</b>	Arachidonate-5 lipoxygenase
<b>ALT</b>	Alanine aminotransferase
<b>ANOVA</b>	Analysis of variance
<b>AP-1</b>	Activator protein-1
<b>ASC</b>	Apoptosis-associated speck-like protein
<b>AST</b>	Aspartate aminotransferase
<b>BBB</b>	Blood-brain barrier
<b>BIOS</b>	Biology-oriented synthesis
<b>BRD4</b>	Bromodomain-containing protein 4
<b>Calc.</b>	Calculated
<b>CASP1</b>	Caspase-1
<b>CDK9</b>	Cyclin-dependent kinase 9
<b>CDCl<sub>3</sub></b>	Deuterated chloroform
<b>CD<sub>3</sub>OD</b>	Deuterated methanol
<b>CDP</b>	Consensus diversity plot
<b>CFA</b>	Complete Freund's adjuvant
<b>CHCl<sub>3</sub></b>	Chloroform
<b>CMAUP</b>	Collective molecular activities of useful plants
<b>CNS</b>	Central nervous system
<b>COCONUT</b>	Collection of open natural products
<b>COSY</b>	Correlation spectroscopy
<b>COX</b>	Cyclooxygenase
<b>COX 1</b>	Cyclooxygenase 1
<b>COX-2</b>	Cyclooxygenase 2
<b>CTRC</b>	Chymotrypsin C
<b>CTSG</b>	Cathepsin G
<b>CYP2D6</b>	Cytochrome P2D6
<b>DCM</b>	Dichloromethane
<b>DMEM</b>	Dulbecco's modified eagle medium
<b>DMSO</b>	Dimethyl sulfoxide
<b>DMSO-d<sub>6</sub></b>	Deuterated dimethyl sulfoxide
<b>DNP</b>	Dictionary of natural products
<b>DOGS</b>	De novo design of generic structures
<b>DOS</b>	Diversity-oriented synthesis

<b>Abbreviation</b>	<b>Full Form</b>
<b>DPPH</b>	2, 2-diphenyl-1-picrylhydrazyl
<b>DTNB</b>	5,5'-dithiobis (2-nitrobenzoic acid)
<b>EGFR</b>	Epidermal growth factor receptor
<b>EIC</b>	Extracted ion chromatogram
<b>eNOS</b>	Endothelial nitric oxide synthase
<b>ERK</b>	Extracellular signal-regulated kinase
<b>ERBB2</b>	Erythroblastic oncogene B homolog 2
<b>ESI-MS</b>	Electrospray ionization-Mass spectrometry
<b>EtOAc</b>	Ethyl acetate
<b>F2</b>	Coagulation factor II
<b>FAME</b>	Fast metabolizer
<b>FASTA</b>	Fast adaptive shrinkage threshold algorithm
<b>FAX</b>	Fatty acid export
<b>FBS</b>	Foetal bovine serum
<b>FLT1</b>	Fms related receptor tyrosine kinase 1
<b>GMQE</b>	Global model quality estimate
<b>GO</b>	Gene ontology
<b>GSH</b>	Glutathione
<b>H-Bond</b>	Hydrogen bond
<b>HEPES</b>	4-(2-hydroxyethyl)-1-piperazineethanesulfonic acid
<b>HeLa</b>	Human cervical cancer cell line
<b>hERG</b>	human ether-a-go-go-related gene
<b>HIA</b>	Human Intestinal Absorption
<b>HMBC</b>	Heteronuclear multiple bond correlation
<b>HPLC</b>	High-performance liquid chromatography
<b>HRMS</b>	High-resolution mass spectrometry
<b>HSQC</b>	Heteronuclear single quantum coherence spectroscopy
<b>HTS</b>	High-throughput screening
<b>HTVS</b>	High-throughput virtual screening
<b>iNOS</b>	Inducible nitric oxide synthase
<b>IC<sub>50</sub></b>	Half-maximal inhibitory concentration
<b>ID<sub>50</sub></b>	Half-maximal infectious dose
<b>IL-1</b>	Interleukin-1
<b>IL-1<math>\beta</math></b>	Interleukin-1 beta
<b>IL-6</b>	Interleukin-6
<b>IL1R1</b>	Interleukin-1 receptor
<b>IKKB</b>	Inhibitor of nuclear factor kappa B kinase subunit beta
<b>JAK1</b>	Janus kinase 1
<b>JNK</b>	c-Jun N-terminal kinase
<b>JNK3</b>	c-Jun N-terminal kinase 3
<b>KDR</b>	Kinase insert domain

<b>Abbreviation</b>	<b>Full Form</b>
<b>KEGG</b>	Kyoto encyclopedia of genes and genomes
<b>KNIME</b>	Konstanz Information Miner
<b>LC-MS</b>	Liquid chromatography-mass spectrometry
<b>LC-QTOF</b>	Liquid chromatography quadrupole time-of-flight
<b>LGA</b>	Lamarckian genetic algorithm
<b>LOX</b>	Lipoxygenase
<b>LPO</b>	Lipid peroxidation
<b>LPS</b>	Lipopolysaccharide
<b>LTA4H</b>	Leukotriene A4 hydrolase
<b>MAPK/ MEK</b>	Mitogen-activated protein kinase
<b>MAPK8</b>	Mitogen-activated protein kinase 8
<b>MD</b>	Molecular dynamic
<b>MDA</b>	Malondialdehyde
<b>MDA-MB-231</b>	Human metastatic breast adenocarcinoma cell line
<b>MEM</b>	Minimum essential medium
<b>MolSA</b>	Molecular surface area
<b>MMP2</b>	Matrix metalloproteinase 2
<b>MM-GBSA</b>	Molecular mechanics-Generalized born surface area
<b>MM-PBSA</b>	Molecular mechanics-Poisson boltzmann surface area
<b>MRSA</b>	Methicillin-resistant <i>Staphylococcus aureus</i>
<b>MS</b>	Mass spectrometry
<b>MTT</b>	3-[4,5-dimethylthiazol-2-yl]-2,5 diphenyl tetrazolium bromide
<b>NCE</b>	New chemical entity
<b>NC-MFP</b>	Natural compound molecular fingerprint
<b>NF-<math>\kappa</math>B</b>	Nuclear factor-kappa B
<b>NLRP3</b>	NLR family pyrin domain containing 3
<b>NMR</b>	Nuclear magnetic resonance
<b>NO</b>	Nitric oxide
<b>NOESY</b>	Nuclear overhauser effect spectroscopy
<b>NOS2</b>	Nitric oxide synthase-2
<b>NP</b>	Natural product
<b>Nrf2</b>	Nuclear factor erythroid 2-related factor 2
<b>NSAID</b>	Non-steroidal anti-inflammatory drugs
<b>NSCLC</b>	Non-small cell lung cancer
<b>PAINS</b>	Pan-assay interference compounds
<b>PBS</b>	Phosphate buffer saline
<b>PDB</b>	Protein data bank
<b>PDBQT</b>	Protein data bank, partial charge (Q), & atom type (T)
<b>PCA</b>	Principal component analysis
<b>PGE2</b>	Prostaglandin E <sub>2</sub>
<b>PGH2</b>	Prostaglandin H <sub>2</sub>

<b>Abbreviation</b>	<b>Full Form</b>
<b>PI3K</b>	Phosphoinositide-3-kinase
<b>PKC</b>	Protein kinase C
<b>PLA2R1</b>	Phospholipase A2 receptor 1
<b>PLC<math>\gamma</math></b>	Phosphoinositide phospholipase C
<b>PMA</b>	Phorbol myristate acetate
<b>PME</b>	Particle mesh ewald
<b>PPB</b>	Plasma protein binding
<b>PPI</b>	Protein-protein interaction
<b>PRKCA</b>	Protein kinase C alpha
<b>PRKCBP1</b>	Protein kinase C binding protein 1
<b>PRKCG</b>	Protein kinase C gamma
<b>PRSS1</b>	Protease serine 1
<b>PSA</b>	Polar surface area
<b>PTGES</b>	Prostaglandin E synthase
<b>PTGES1</b>	Prostaglandin E synthase 1
<b>PTGES2</b>	Prostaglandin E synthase 2
<b>PWF</b>	Paw withdrawal frequency
<b>PWL</b>	Paw withdrawal latency
<b>PWT</b>	Paw withdrawal threshold
<b>Rg/RoG/rGyr</b>	Radius of gyration
<b>RMSD</b>	Root mean square deviation
<b>RMSF</b>	Root mean square fluctuation
<b>ROCS</b>	Rapid overlay of chemical structures
<b>Ro5</b>	Rule of five
<b>ROS</b>	Reactive oxygen species
<b>SAR</b>	Structure-activity relationship
<b>SASA</b>	Solvent-accessible surface area
<b>SB-DFP</b>	Statistical-based database fingerprint
<b>SCLC</b>	Small cell lung cancer
<b>SD</b>	Standard deviation
<b>SDS</b>	Sodium dodecyl sulphate
<b>SEM</b>	Standard error mean
<b>SHB</b>	SH2 domain containing adaptor protein B
<b>SL</b>	Sesquiterpene lactone
<b>SRC</b>	Proto-oncogene tyrosine-protein kinase
<b>SP</b>	Standard precision
<b>SPiDER</b>	Self-organizing map-based prediction of drug equivalence relationships
<b>STarFish</b>	Stacked ensemble target fishing
<b>STAT3</b>	Signal transducer and activator of transcription 3
<b>TAK1</b>	Transforming growth factor- $\beta$ (TGF- $\beta$ )-activated kinase 1
<b>TBA</b>	Thio barbituric acid

<b>Abbreviation</b>	<b>Full Form</b>
<b>TBARS</b>	Thiobarbituric acid reactive substances
<b>TBX2</b>	T-Box transcription factor 2
<b>TCM</b>	Traditional Chinese Medicine
<b>TIP3P</b>	Transferable intermolecular potential with 3 points
<b>TLC</b>	Thin-layer chromatography
<b>TMS</b>	Tetramethylsilane
<b>TNB</b>	Thionitro benzoic acid
<b>TNF-<math>\alpha</math></b>	Tumor necrosis factor- $\alpha$
<b>TNBC</b>	Triple-negative breast cancer
<b>t-SNE</b>	T-distributed stochastic neighbor embedding
<b>TIGER</b>	Target inference generator
<b>TSAd</b>	T cell-specific adapter protein
<b>UMAP</b>	Uniform manifold approximation and projection
<b>US FDA</b>	United States Food & Drug administration
<b>UV</b>	Ultraviolet
<b>VEGFs</b>	Vascular endothelial growth factors
<b>VEGFRs</b>	Vascular endothelial growth factor receptors
<b>VEGFR-2</b>	Vascular endothelial growth factor receptor- 2
<b>VISA</b>	Vancomycin-intermediate <i>Staphylococcus aureus</i>
<b>VRE</b>	Vancomycin-resistant <i>Enterococci</i>
<b>XP-</b>	Extra precision
<b>XRD</b>	X-ray diffraction
<b>YES1</b>	YES proto-oncogene 1

## List of Symbol

<b>Symbols</b>	<b>Meaning</b>
$\alpha$	Alpha
$\beta$	Beta
$\gamma$	Gamma
$\delta$	Delta
$\omega$	Omega
~	Approximately
Å	Angstrom
$\kappa$	Kappa
$\pm$	Plus or Minus
<	Less than
>	Greater than
$\geq$	Greater than equal to
$\leq$	Less than or equal to
%	Percent
$\mu\text{M}$	Micromolar
$\text{nM}$	Nanomolar
$\text{mM}$	Millimolar
$\mu\text{L}$	Microliter
$\text{mL}$	Milliliter
L	Liter
$\mu\text{g/mL}$	Micrograms per milliliter
pH	Potential of hydrogen
K	Kelvin
ns	Nanosecond
ps	Picosecond
$\text{kcal/mol}$	Kilocalories per mole
nm	Nanometer
sec	Second
min	Minute
hr	Hour
Hz	Hertz
MHz	Megahertz
J	Coupling constant
ppm/ $\delta$	Parts per million
s	Singlet
d	Doublet
t	Triplet
dd	Doublet of doublet
dt	Doublet of triplet
m	Multiplet

<b>Symbols</b>	<b>Meaning</b>
<b>m/z</b>	Mass-to-charge ratio
<b>mg</b>	Milligrams
<b>mg/dl</b>	Milligrams per deciliter
<b>g</b>	Grams
<b>kg</b>	Kilograms
<b>mg/kg</b>	Milligrams per kilogram
<b>rpm</b>	Revolutions per minute
<b>i.p.</b>	Intraperitoneal