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Collective In Silico Studies Reveal Bioactive Compounds from Sea Grapes (Caulerpa lentillifera) Target p38 MAPK for Potential Anti Aging Applications
Haiva Kezia, Dr. Sci. apt. Rohmad Yudi Utomo, M.Sc.
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LIST OF ABBREVIATIONS

ADMET	: Absorption, Distribution, Metabolism, Excretion, and Toxicity
AKT	: Protein Kinase B
AP-1	: Activator Protein 1
Arg	: Arginine
Asp	: Aspartic Acid
ATP	: Adenosine Triphosphate
AUC	: Area Under the Curve
BBB	: Blood-Brain Barrier
BOILED-Egg	: Brain Or IntestinaL EstimateD permeation method
CNS	: Central Nervous System
DC	: Dendritic Cell
DFG	: Aspartate-Phenylalanine-Glycine
DNA	: Deoxyribonucleic Acid
ECM	: Extracellular Matrix
ESI	: Electrospray Ionization
ESOL	: Estimated Solubility
GHS	: Globally Harmonized System of Classification and Labelling of Chemicals
GI	: Gastrointestinal
Glu	: Glutamic Acid
HBA	: Hydrogen Bond Acceptor
HBD	: Hydrogen Bond Donor

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His	: Histidine
HPLC	: High-Performance Liquid Chromatography
HRD	: Histidine-Arginine-Aspartate
HRMS	: High-Resolution Mass Spectrometry
Ile	: Isoleucine
KE1	: Protein Reactivity
KE2	: KeratinoSens
KE3	: DC Activation
KE4	: T-Cell Activation
KE5	: Final Adverse Outcome
KEGG	: Kyoto Encyclopedia of Genes and Genomes
KNIME	: Konstanz Information Miner
Leu	: Leucine
log KP	: Logarithm of Skin Permeability Coefficient
logP	: Logarithm of Octanol-Water Partition Coefficient
Lys	: Lysine
MACCS	: Molecular Accelrys Keys / Molecular Design Limited Public Keys
MAPK	: Mitogen-Activated Protein Kinase
Met	: Methionine
MLP	: Multilayer Perceptron
MMP	: Matrix Metalloproteinase
MMP1	: Matrix Metalloproteinase 1
MMPs	: Matrix Metalloproteinases

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MOE	: Molecular Operating Environment
MS	: Mass Spectrometry
mTOR	: Mechanistic Target of Rapamycin
MW	: Molecular Weight
NF-kappa B	: Nuclear Factor Kappa Light Chain Enhancer of Activated B Cells
NPASS	: Natural Product Activity and Structural Database
P38 MAPK	: p38 Mitogen-Activated Protein Kinase
P-gp/Pgp	: P-glycoproteinp-38
MAPK	: Mitogen-Activated Protein Kinase
PDB	: Protein Data Bank
Phe	: Phenylanine
PKS	: Polyketide Synthase
PRED-Skin	: Prediction of Human Skin Sensitizers
RAS	: Rat Sarcoma
RCS	: Reactive Chlorine Species
RDKit	: Rational Discovery Kit (Cheminformatics and Machine Learning Software Toolkit)
RF	: Random Forest
RMSD	: Root-Mean-Square Deviation
RNS	: Reactive Nitrogen Species
Ro5	: Rule of Five
ROC	: Receiver Operating Characteristic
ROS	: Reactive Oxygen Species

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S	: docking score
SASP	: Senescence-Associated Secretory Phenotype
SMILES	: Simplified Molecular-Input Line-Entry System
SVM	: Support Vector Machine
Thr	: Threonine
TPSA	: Topological Polar Surface Area
UHPLC-MS	: Ultra-High Performance Liquid Chromatography-Mass Spectrometry
UV	: Ultraviolet
Val	: Valine