KOMBAT: Knowledgebase of Microbes’ Battling Agents for Therapeutics

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Supplementary Table 1: List of antimicrobial databases retrieved from literature

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| --- | --- | --- | --- | --- |
| Category | Name | Database focus | Link | PMID |
| Antimicrobial peptide database | PhytAMP | Antimicrobial plant peptides | https://webs.iiitd.edu.in/raghava/satpdb/catalogs/phytamp/ | 18836196 |
| DBAASP | Chemical, 3D structure and activity for experimentally evaluated antimicrobial peptides | https://dbaasp.org/ | 24888447 |
| APD | Antibacterial, antifungal, antiviral and antitumor peptides | https://aps.unmc.edu/ | 14681488 |
| CAMPR3 | Sequences, structures and signatures of antimicrobial peptides | http://www.camp.bicnirrh.res.in/ | 26467475 |
| DRAMP | Repository of general AMPs, patented sequences and peptides in drug development | http://dramp.cpu-bioinfor.org/ | 27075512 |
| AntiTbPdb | Experimentally validated anti-tubercular peptides compiled from literature | https://webs.iiitd.edu.in/raghava/antitbpdb/ | 29688365 |
| AVPdb | Experimentally validated antiviral peptides | https://webs.iiitd.edu.in/raghava/satpdb/catalogs/avpdb/ | 24285301 |
| ParaPep | Experimentally validated antiparasitic peptide sequences and their structures | https://webs.iiitd.edu.in/raghava/parapep/help.php | 24923818 |
| DADP | Manually curated database of antimicrobial and other defense peptides from frog | http://split4.pmfst.hr/dadp/ | 22467909 |
| BaAMPs | Biofilm-active antimicrobial peptides | http://www.baamps.it/ | 25760404 |
| LAMP | Antimicrobial peptide with information about their antimicrobial activity and cytotoxicity | http://biotechlab.fudan.edu.cn/database/lamp/ | 23825543 |
| BACTIBASE | Bacteriocins with activity against various human and animal pathogens | http://bactibase.hammamilab.org/main.php | 17941971 |
| THPdb | FDA-approved peptide and protein therapeutics | https://webs.iiitd.edu.in/raghava/thpdb/keyword.php | 28759605 |
| PlantAFP | Plant-origin antifungal peptides | http://bioinformatics.cimap.res.in/sharma/PlantAFP/ | 31612325 |
| MimoDB | Pepository for therapeutic peptides | https://dbpedia.org/page/MimoDB | 21079566 |
| YADAMP | Antimicrobial peptides from all biological sources active against bacteria. | https://webs.iiitd.edu.in/raghava/satpdb/catalogs/yadamp/ | 22325123 |
| Molecule | AntibioticDB | Clinically relevent antibacterial compounds | https://antibioticdb.com/ | 29897476 |
| ChemDB | Database of small molecules and related chemoinformatics resources | http://chemdb.ics.uci.edu/ | 16174682 |
| ASDCD | Antifungal synergistic drug combination | http://asdcd.amss.ac.cn/ | 24475134 |
| DenvInD | Dengue virus inhibitors database | https://webs.iiitd.edu.in/raghava/denvind/ | 32510549 |
| Drug Target | TDD | Known therapeutic protein and nucleic acid targets described in the literature | http://db.idrblab.net/ttd/ | 11752352 |
| PfalDB | Drug target and chemical database for Plasmodium falciparum | http://indirag.org/database/3 | 25198774 |
| Clostridium-DTDB | Rotential drug targets with their structural information from Clostridium difficile | http://clostridium.bicpu.edu.in/ | 23415847 |
| sc-PDB | Three-dimensional structures of druggable binding sites | http://bioinfo-pharma.u-strasbg.fr/scPDB/ | 16563002 |
| Gene/ Sequence | CARD | Database of resistance genes, their products and associated phenotypes | https://card.mcmaster.ca/ | 23650175 |
| MEGARes | High-Throughput Sequencing database | https://megares.meglab.org/ | 27899569 |
| VFDB | Database of virulence factors of bacterial pathogens | http://www.mgc.ac.cn/VFs/ | 15608208 |
| PATRIC | Consistent annotations across all sequenced bacterial species | https://www.patricbrc.org/ | 24225323 |
| Mustard | Antimicrobial resistance genes and AR Determinants | http://mgps.eu/Mustard/ | 30478291 |
| BacMet | antibacterial biocide and metal resistance genes | http://bacmet.biomedicine.gu.se/ | 24304895 |
| MARDy | Database of antifungal drug resistance mechanisms, including amino acid substitutions, tandem repeat sequences and genome ploidy | http://www.mardy.net/ | 29897419 |
| FARME DB | Functional metagenomic antibiotic resistance (AR) gene elements | http://staff.washington.edu/jwallace/farme/ | 28077567 |
| u-CARE | Antibiotics with reported resistance, 107 genes, transcription factors and single nucleotide polymorphism (SNPs) involved in multiple drug resistance | http://www.e-bioinformatics.net/ucare/ | 25935546 |
| ARDB | Annotation of gene and resistance type | https://ardb.cbcb.umd.edu/ | 18832362 |

\*Accessibility was manually checked and only resources with active link were included in the link.

Supplementary Table 2: Word Combinations used in the subjective (sentimental) approach

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| --- | --- |
| TERM1 | TERM2 |
| Alternative | Acceptable, Advance, Affordable, Agent, Allosteric, Appealing, Applicable, Application, Approach, Appropriate, Assay, Beneficial, Best, Biocide, Bioactive, Biocidal, Candidate, Chemo, Choice, Combination, Compensatory, Compound, Derivative, Diagnos, Effective, Efficient, Eradication, Evidence, Finding, Helpful, Herbal, Inhibitor, Measure, Method, Molecule, Optimal, Option, Possible, Potent, Product, Rational, Reasonable, Relevent, Satisfactory, Selective, Sensitive, Solution, Source, Strategy, Substituent, Success, Suitable, Synthetic, Technique, Technology, Therapeutic, Therapy, Treatment, Unique, Useful, Valuable |
| Alternate | Agent, Choice, Dose, Mode, Route, Solution, Source, Strategy, Therapeutic , Treatment |
| Potent | Activity, Adjunctive, adjuvant, Analogue, Antagonist, Antiinfective, Bactericide, Better, Candidate, Chemical, Chemotherapy, Clinical, Compound, Confer, Conjugate, Demonstrate, Derivative, Design, Develop, Display, Elicit, Endow, Equal, Especial, Exceptional, Exert, Exhibit, Herbal, Highly, Immunosuppressant, Increasing, Inducer, Inhibitor, Molecule, Most, Natural, New, Novel, Pharmacodynamic, Phytochemical, Phytotherapeutic, Predict, Promising, Prove, Regimen, Remark, Reveal, Show, Significant, Source, Substance, Synthetic, Therapy, Unique, Very ,Wide |
| Prevent | Accept, Acquire, Action, Activ, Additional, Adjunctive, Adjuvant, Administration, Adopt, Advice, Against, Agent, Alternate, Alternative, Antibiotherapy, Appeal, Application, Approach, Appropriate, Aspect, Attractive, Available, Behavioral, Benefit, Best, Better, Center, Chemo, Concept, Conclusion, Concomitant, Condition, Contain, Control, Current, Define, Design, Despite, Develop, Diagnostic, Effect, Efficient, Effort, Especial, Establish, Evaluation, Exert, Extensive, Guide, Ideal, Identify, Immun, Impact, Implement, Important, Improve, Include, Induce, Infect, Inform, Initiative, Innovative, Intensive, Interest, Intermittent, Intervention, Isolate, Local, Measure, Medicine, Method, Multimodal, National, Neglect, New, Nonpharmacologic, Novel, Optimal, Optimize, Personalised, Policy, Possible, Potent, Powerful, Practice, Prescribe, Present, Presume, Primary, Principle, Probiotic, Procedure, Program, Promising, Proper, Propose, Protect, Protocol, Provide, Purpose, Rank, Rational, Receive, Recommend, Regimen, Service, Significant, Special, Specific, Strategy, Target, Tech, Term, Test, Therapeutic, Therapy, Tool, Transmission, Treatment, Trial |
| Next | Available, Best, Challenge, Common, Compare, Complementary, Correct, Couple, Critical, Decade, Demonstrate, Design, Develop, Direct, Discover, Domain, Effective, Episode, Evaluate, Exacerbation, Examine, Experiment, Favourable, Generation, Goal, Improve, Infection, Inhibitor, Inoculum, Investigate, Nucleotide, Observation, Occurrence, Opportunity, Organism, Orientation, Phase, Pivotal, Position, Potent, Predominant, Promising, Pseudodiphtheriticum, Recurrence, Regimen, Region, Research, Resistant, Route, Sample, Screen, Stage, Strand, Strategy, Study, Successful, Synthesize, Test, Therapeutic, Treatment, Use, Utilize, Validate |
| Strategy | Acceptable, Acclimation, Accurate, Activation, Adapt, Additional, Adjuvant, Advance, Advocate, Aeration, Afford, Against, Agent, Aggressive, Analytic, Anticipating, Anticontamination, Antioxidant, Antipersister, Antisense, Appealing, Appear, Application, Apply, Approach, Appropriate, Asses, Associat, Attractive, Avert, Avoid, Base, Basic, Behavioral, Benchmark, Beneficial, Best, Better, Bioassay, Biochemical, Biofilm, Biomarker, Biomimick, Bioremediation, Biosensing, Biosynthetic, Challeng, Chandross, Change, Chemical, Chemo, Chosen, Class, Clear, Clinical, Cocktail, Coinfection, Collaborative, Common, Community, Compare, Complement, Component, Compose, Comprehensive, Computation, Concern, Condensation, Conservative, Consistent, Control, Coordinate, Counterproductive, Counterselection, Couple, Critical, Crowdsourcing, Current, Cycling, Decision, Decolonization, Deconvolution, Deescalation, Defense, Define, Demand, Demonstrate, Depend, Derive, Desensitization, Deserve, Design, Detect, Deterioration, Detoxify, Develop, Devising, Devote, Diagnostic, Direct, Discontinuation, Discovery, Disruption, Dissemination, Diversification, Dominant, Driven, Ecological, Effective, Efficient, Electrochemical, Elimination, Emerge, Emptive, Encourag, Enhance, Entail, Escalat, Escape, Especial, Essential, Establish, Evolutionary, Excellent, Exchange, Excision, Excit, Expensive, Experiment, Exploit, Exposure, Extreme, Fast, Feasible, Feedback, Focus, Footprinting, Formulation, Fundamental, Global, Glycodiversification,Heterogeneity, Hierarchic, Hybrid, Ideal, Identifie, Immobilization, Immunization, Immunoenzymatic, Immunomodulatory, Immunotherapeutic, Implement, Implies, Important, Improve, Inactivation, Incentive, Infect, Inference, Inhibit, Initial, Initiation, Innovative, Integrat, Intensification, Intensive, Interest, Interim, Interpretation, Interruption, Intervention, Intriguing, Invasion, Invasive, Inverse, Investigation, Lead, Liberal, Loss, Lysis, Microfluidic, Mimetic, Mitigat, Model, Multi, Mycobacterial, Nanotech, National, Need, Opposite, Optim, Particular, Personal, Pharma, Phase, Physiological, Phytotherapeutic, Plausible, Pluridisciplinary, Popular, Possible, Potent, Powerful, Practical, Predict, Prefer, Prescrib, Prevent, Primary, Proactive, Probe, Probiotic, Prodrug, Produce, Product, Progressive, Promising, Proof, Proper, Prophyla, Protect, Radioactive, Reasonable, Relevant, Replacement, Replication, Report, Represent, Require, Rescue, Research, Resist, Resolution, Resource, Revascularization, Risk, Robust, Simple, Solution, Specific, Standard, Straightforward, Strong, Success, Suggest, Suitable, Superior, Supplement, Support, Surgical, Surrogate, Surveillance, Survival, Sustain, Synerg, Synthesis, Synthetic, Systematic, Target, Traditional, Transcomplementation, Transcription, Transduction, Transfer, Transformation, Translation, Treat, Trial, Ultimate, Undefined, Underlying, Underutilized, Unexplore, Unique, Universal, Unprecedent, Untenable, Use, Utiliz, Valid, Valuable, Versatile, Viable, Virulence, Vital |
| Novel | Adjunct, Adjuvant, Agent, Analog, Antibiofilm, Application, Approach, Arrangement, Assay, Bactericidal, Bacteriocin, Bioactive, Biosynthetic, Candidate, Chemical, Chemo, Class, Combination, Complex, Component, Composit, Compound, Concept, Conjugate, Idea, Immuno, Inhibitor, Lead, Ligand, Measure, Mechanism, Mediator, Method, Microbiological, Microparticle, Mode, Molecule, Nano, Natural, Observation, Peptide, Pharmaceutical, Potential, Powerful, Probiotic, Process, Product, Result, Solution, Source, Substance, Substituent, Synthetic, System, Target, Technique, Technology, Therapy, Treatment, Type, Unexploited, Unique, Valuable, Variant, Vision, Way |
| New | Addition, Adjuvant, Alternative, Antagonist, Antiadhesion, Antioxidant, Approach, Avenue, Bactericidal, Bacteriocin, Bioactive, Biocidal, Biocide, Biocompatible, Biodetergent, Biofilm, Biohybrid, Bioisosteres, Biomaterial, Biosynthetic, Chemical, Chemotype, Choice, Class, Combination, Composite, Concept, Conjugate, Cure, Development, diagnose, Dipeptide, Effective, Efficient, Element, Emergence, Enhance, Evidence, Extract, Finding, Formulation, Fusion, Genera, Herbal, Idea, Inhibitor, Innovation, Insight, Knowledge, Lead, Material, Measure, Method, Molecule, Nanoparticle, Natural, Observation, Opportunity, Option, Peptide, Plant, Potent, Predict, Probiotic, Product, Promising, Remedy, Resource, Result, Significant, Solution, Source, Strategy, Structure, Study, Substance, Substitution, Substrate, Synthetic, Technique, Technology, Therapeutic, Variant, Vision, Way |
| Promising | Adjunctive, Adjuvants, Agent, Alternative, Application, Approach, Area, Assay, Avenue, Bactericidal, Basis, Biocidal, Biomaterial, Biotechnology, Candidate, Chemical, Chemotherapeutic, Class, Combination, Compound, Concept, Derivative, Diagnostic, Drug, Effect, Efficacy, Extract, Formulation, Herbal, Hit, Inhibitor, Innovation, Lead, Material, Method, Molecule, Natural, Opportunity, Option, Peptide, Platform, Potency, Potent, Preventive, Probiotic, Protocol, Regimen, Result, Route, Solution, Source, Strategy, Substitute, Target, Technique, Technology, Template, Therapeutic, Tool, Treatment, Way |
| Therapeutic | Adequate, Adjuvant, Alternative, Approve, Bacteriophage, Beneficial, Better, Biocompatible, Biofilm, Biological, Biosensing, Cell, Challenge, Complementary, Develop, Effective, Efficacious, Experiment, Future, Glycopeptide, Improve, Inhibitor, Innovative, Investigational, Multicomponent, Natural, New, Novel, Peptide, Polymer, Potential, Powerful, Probiotic, Rational, Silver, Valuable |
| Therapy | Adequate, Adjunct, Adjuvant, Aerosol, Alternate, Alternative, Another, Antimicrobial, , Antioxidant, Appropriate, Assisted, Backup, Bacteria, Based, Combination, Common, Concomitant, Concordant, Conventional, Definitive, Diagnostics, Different, Directed, Effective, Efficient, Endodontic, Emerge, Extended, Flipside, Future, Gene, Guiding, Hybrid, Ideal, Improve, Independent, Induction, Infective, Inhibitor, Initial, Interval, Leech, Line, New, Novel, Novo, Optimal, Oxygen, Phage, Photodynamic, Precise, Probiotic, Prolong, Promising, Radiation, Replacement, Rescue, Second, Sequential, Substitute, Supportive, Suppressant, Surrogate, Synergistic, Systemic, Tailored, Target, Topical, Traditional, Virulence |