**Supplementary Materials**

**S1. Table of AI-First Drug Discovery Companies**

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| --- | --- | --- | --- | --- |
| Company | Target | Disease | Compound | Status |
| BenevolentAI | TRKHRH3PDE10UndisclosedUndisclosed | Atopic DermatitisNarcolepsyUlcerative ColitisGM~~1~~ALS~~1~~ | BEN-2293BEN-2001BEN-8744BEN-28010BEN-34712 | DiscontinuedDiscontinuedPreclinicalPreclinicalPreclinical |
| Relay Therapeutics | PI3KαPI3KαFGFR2SHP2 | Breast CancerBreast CancerSolid TumorsSolid Tumors | RLY-5836RLY-2608RLY-4008GDC-1971 | Phase 1Phase 1Phase 1/2Phase 1 |
| GV20 Therapeutics | IGSF8 | Solid Tumors | GV20-0251 | Phase 1 |
| Celsius Therapeutics | TREM1 | IBD~~1~~ | CEL-383 | Phase 1 |
| Neumora | KORV1aRM4RNMDACK1δNLRP3GCASE | Depression/NPD~~1~~Alzheimer’s/PTSD~~1~~SchizophreniaSchizophreniaALS~~1~~/Parkinson’sParkinson’sParkinson’s | NMRA-140NMRA-511NMRA-M4RNMRA-NMDANMRA- CK1δNMRA-NLRP3NMRA-GCASE | Phase 2/3Phase 1PreclinicalPreclinicalPreclinicalPreclinicalPreclinical |
| Insilico Medicine | UndisclosedUSP1 | Kidney Fibrosis/IPF~~1~~Breast Cancer | INS-018\_055ISM-3091 | Phase 2Phase 1 |
| Evaxion | NeoantigenNeoantigenNeoantigen NSaA1~~2~~NNgA1~~2~~ | MelanomaMelanomaLung cancer*S. aureus* *N. gonorrhoeae* | EVX-01EVX-02EVX-03EVX-B1EVX-B2 | Phase 2Phase 1/2PreclinicalPreclinicalPreclinical |
| Athos | UndisclosedUndisclosedUndisclosed | IBD~~1~~IBD~~1~~IBD~~1~~ | ATH-063ATH-105ATH-131 | Phase 1PreclinicalPreclinical |
| OrphAI | C9ORF72mTORUndisclosedmTOR | ALS~~1~~PAH~~1~~BO~~1~~PS~~1~~ | AIT-101LAM-001LAM-001LAM-001 | Phase 2Phase 2Phase 2Phase 1 |
| Accutar | ERERARBTK | Breast CancerBreast CancerProstate CancerBlood Cancer | AC-0699AC-0682AC-0176AC0676 | Phase 1Phase 1Phase 1Phase 1 |
| Schrödinger | IDH1MALT1CDC7CDC7 | AML~~1~~NHL~~1~~Blood CancerSolid Tumor  | AG-120SGR-1505SGR-2921SGR-2921 | Approved~~3~~2Phase 1Phase 1Phase 1 |
| Exscientia | CDK7PKCθLSD1 MALT1A2A | Solid Tumor ID~~1~~AML~~1~~Blood CancerKidney/Lung Cancer | GTAEXS-617EXS-4318EXS-74539EXS-73565EXS-21546 | Phase 1/2Phase 1/2 PreclinicalPreclinicalDiscontinued |
| Recursion | UndisclosedNF2APCAXIN1UndisclosedRBM39GM2 | CCM~~1~~Brain CancerFAP~~1~~Solid Tumor*C. difficile* Ovarian CancerGangliosidosis | REC-994REC-2282REC-4881REC-4881REC-3964UndisclosedREC-3599 | Phase 2Phase 2Phase 2Phase 1Phase 1PreclinicalDiscontinued |
| Totus Medicines | PI3KCA | Solid Tumors | TOS-358 | Phase 1 |
| Calico | TDP43UndisclosedUndisclosed | ALSSolid TumorSolid Tumor | ABBV-CLS-7262ABBV-CLS-484ABBV-CLS-579 | Phase 1Phase 1Phase 1 |
| Biolojic Design | IL2IL13 / TSLPIL2 | Solid Tumor Solid TumorSolid Tumor | AU-007BD-9BD-3 | Phase 1PreclinicalPreclinical |
| BPG Bio  | UndisclosedUndisclosedUndisclosedUndisclosedUndisclosedUndisclosed | Epidermolysis BullosaCIA~~1~~Sarcopenia SCC~~1~~Pancreatic CancerGM~~1~~ | BPM-31510BPM-31510BPM-31510BPM-31510BPM-31510BPM-31510IV-11 | Phase 1Phase 1Phase 1Phase 2Phase 2Phase 2 |
| Auransa | UndisclosedUndisclosed | Liver CancerHeart-Safe Chemo | AU-409AU-018 | Phase 1Preclinical |
| Invea Therapeutics | CMA1CMA1CMA1CARD55HT2~~3~~ | Atopic DermatitisChronic UrticariaISM~~1~~ID~~1~~IBD~~1~~ | INVA-8001INVA-8001INVA-8001INVA-8003INVA-8002 | Phase 1PreclinicalPreclinicalPreclinicalDiscontinued |
| Bullfrog AI  | UndisclosedUndisclosed | GlioblastomaGlioblastoma | BF-222BF-223 | Phase 1Preclinical |
| Pharos iBio | UndisclosedUndisclosedUndisclosedRAF/DDR | AML~~1~~Ovarian CancerBreast CancerSolid Tumor  | PHI-101PHI-101PHI-101PHI-501 | Phase 1PreclinicalPreclinicalPreclinical |
| Nimbus Therapeutics | HPK1 | Solid Tumor  | NDI-101150 | Phase 1/2 |
| BioXcel Therapeutics | Alpha-2Alpha-2Alpha-2Alpha-2 Undisclosed | Schizophrenia/BPD~~1~~Alzheimer’sSchizophrenia/BPDDepressionAlzheimer’s | DexmedetomidineBXCL-501BXCL-501BXCL-501BXCL-502 | ApprovedPhase 3Phase 3Phase 1Preclinical |
| Ideaya Biosciences | PKCMAT2APARGPOLQWRN | Uveal MelanomaSolid TumorBreast/Ovarian CancerSolid TumorGastrointestinal Cancer | DarovartesibIDE-397IDE-161GSK-101WRN | Phase 2/3Phase 1Phase 1PreclinicalPreclinical |
| Roivant Sciences | AhRAhRTL1ATL1AFcRnFcRnFcRnFcRnTYK2/JAK1TYK2/JAK1CSF2SF3B1 | PsoriasisAtopic DermatitisUlcerative ColitisCrohn’s DiseaseMyasthenia GravisThyroid Eye DiseaseWAIHA~~1~~Autoimmune DiseaseDermatomyositisSLE~~1~~SarcoidosisMDS | TapinarofTapinarofRVT-3101RVT-3101BatoclimabBatoclimabBatoclimabIMVT-1402BrepocitinibBrepocitinibNamilumabRVT-2001 | ApprovedPhase 3Phase 3Phase 2Phase 3Phase 2Phase 1Phase 1Phase 3Phase 2Phase 2Phase 1 |

Table S1: Targets identified and under development in AI-first biopharmaceutical companies. Targets and compound identifiers are being queried from company pipelines and ClinicalTrials.gov.

~~1~~GM = Glioblastoma Multiforme; ALS = Amyotrophic lateral sclerosis; IBD = Inflammatory Bowel Disease; NPD Neuropsychiatric Disorders; PTSD = Post-Traumatic Stress Disorder; IPF = Idiopathic Pulmonary Fibrosis; PAH = Pulmonary Arterial Hypertension; BO = Bronchioliti~~t~~s Obliterans; PS = Pulmonary Sarcoidosis; AML = Acute Myeloid Leukemia; NHL = Non-Hodgkin Lymphoma; ID = Inflammatory Disease; CCM = Cerebral Cavernous Malformation; FAP = Familial Adenomatous Polyposis; CIA = Chemotherapy-induced Alopecia; SCC = Squamous Cell Carcinoma; ISM = Indolent Systemic Mastocytosis ; CN = Cutaneous Neurofibroma; BPD = Bipolar Disorder; WAIHA = Warm Autoimmune Hemolytic Anemia; SLE = Systemic Lupus Erythematosus; MDS = Myelodysplastic Syndromes.

1~~2~~NSaA = Novel *S. aureus* Antigens; NNgA = Novel *N. gonorrhoeae* Antigens

2~~3~~In collaboration with Agios Pharmaceuticals. Acquired by Servier.

**S2. Database Citations**

In order of appearance in Table 1: UK Biobank (Bycroft *et al.* 2018), Genes & Health (Finer *et al.* 2020), OpenTargets (Ochoa *et al.* 2021), TCGA (Weinstein *et al.* 2013), GEO (Clough and Barrett 2016), GO (Ashburner *et al.* 2000), Ensembl (Martin *et al.* 2023), UniProt (The UniProt Consortium 2023), UCSC Genome Browser (Kent *et al.* 2002), ChEMBL (Mendez *et al.* 2019), GenBank (Sayers *et al.* 2021), PDB (Berman *et al.* 2000), GENCODE (Frankish *et al.* 2021)

STRING (Szklarczyk *et al.* 2023), STITCH (Kuhn *et al.* 2008), BioGRID (Stark *et al.* 2006), TRRUST (Han *et al.* 2018), RegNetwork (Liu *et al.* 2015), IntAct (Kerrien *et al.* 2007), Reactome (Gillespie *et al.* 2022), KEGG (Kanehisa *et al.* 2023), TCIA (Clark *et al.* 2013), GDC (Grossman *et al.* 2016),MICA-MIC (Royer *et al.* 2022)