high throughput screening

	NCT Number	Title	Authors	Description	Identifier	Dates
1	pubmed:36088848	Direct introduction MALDI FTICR MS based on dried droplet deposition applied to non-targeted metabolomics on Pisum Sativum root exudates	Valentina Calabrese Isabelle Schmitz-Afonso Wassila Riah-Anglet Isabelle Trinsoutrot-Gattin Barbara Pawlak Carlos Afonso	Non-targeted metabolomic approaches based on direct introduction (DI) through a soft ionization source are nowadays used for large-scale analysis and wide cover-up of metabolites in complex matrices. When coupled with ultra-high-resolution Fourier-Transform ion cyclotron resonance (FTICR MS), DI is generally performed through electrospray (ESI), which, despite the great analytical throughput, can suffer of matrix effects due to residual salts or charge competitors. In alternative, matrix	pmid:36088848 doi:10.1016/j.talanta.2022.123901	Sun, 11 Sep 2022 06:00:00 -0400
2	pubmed:36089166	The larval diving response (LDR): validation of an automated, high-throughput, ecologically relevant measure of anxiety-related behavior in larval zebrafish (Danio Rerio)	Barbara D Fontana Matthew O Parker	CONCLUSIONS: This new automated and high-throughput screening tool has the potential use for screening of anxiogenic and anxiolytic compounds, and for studies aiming to better understand anxiety-like behaviors.	pmid:36089166 doi:10.1016/j.jneumeth.2022.109706	Sun, 11 Sep 2022 06:00:00 -0400
3	pubmed:36089219	Sequence-based Functional Metagenomics Reveals Novel Natural Diversity of Functioning CopA in Environmental Microbiomes	Wenjun Li Likun Wang Xiaofang Li Xin Zheng Michael F Cohen Yong-Xin Liu	Exploring the natural diversity of functional genes/proteins from environmental DNA in high-throughput remains challenging. In this study, we developed a sequence-based functional metagenomics procedure for mining the diversity of copper resistance gene copA in global microbiomes, by combining the metagenomic assembly technology, local BLAST, evolutionary trace analysis (ETA), chemical synthesis, and conventional functional genomics. In total, 87 metagenomes were collected from a public database	pmid:36089219 doi:10.1016/j.gpb.2022.08.006	Sun, 11 Sep 2022 06:00:00 -0400
4	pubmed:36089246	A Perspective on the Discovery of Enzyme Activators	Antonia Turberville Hannah Semple Gareth Davies Delyan Ivanov Geoffrey A Holdgate	Enzyme activation remains a largely under- represented and poorly exploited area of drug discovery despite some key literature examples of the successful application of enzyme activators by various mechanisms and their importance in a wide range of therapeutic interventions. Here we describe the background nomenclature, present the current position of this field of drug discovery and discuss the challenges of hit identification for enzyme activation, as well as our perspectives on the approaches	pmid:36089246 doi:10.1016/j.slasd.2022.09.001	Sun, 11 Sep 2022 06:00:00 -0400
5	pubmed:36089324	A microfluidic droplet array demonstrating high-throughput screening in individual lipid-producing microalgae	Guoxia Zheng Furong Gu Yutong Cui Ling Lu Xuejun Hu Lin Wang Yunhua Wang	Microalgae are a group of photoautotrophic microorganisms which could use carbon dioxide for autosynthesis. They have been envisioned as one of the most prospective feedstock for renewable oil. However, great endeavors will still be needed to increase their economic feasibility. The screening of competitive species and suitable culture conditions are such issues. To greatly accelerate these rather laborious steps and also improve their experimental lump-summanner, we developed a microfluidic	pmid:36089324 doi:10.1016/j.aca.2022.340322	Sun, 11 Sep 2022 06:00:00 -0400

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6	pubmed:36089663	Micropatterned Hydrogels with Highly Ordered Cellulose Nanocrystals for Visually Monitoring Cardiomyocytes	Junmei Wang Qian Liu Jixing Gong Zhongjun Wan Jinping Zhou Chunyu Chang Donghui Zhang	Cardiac microphysiological systems are accurate in vitro platforms that reveal the biological mechanisms underlying cardiopathy, accelerating pharmaceutical research in this field. Current cardiac microphysiological devices and organs-on-chips consist of several layers prepared with complex, multi-step processes. Incorporating inorganic photonic crystals may cause long-term biocompatibility issues. Herein, micropatterned hydrogels with anisotropic structural colors are prepared by locking	pmid:36089663 doi:10.1002/smll.202202235	Sun, 11 Sep 2022 06:00:00 -0400
7	pubmed:36090047	A Fe ²⁺ -dependent self-inhibited state influences the druggability of human collagen lysyl hydroxylase (LH/PLOD) enzymes	Luigi Scietti Elisabetta Moroni Daiana Mattoteia Marco Fumagalli Matteo De Marco Lisa Negro Antonella Chiapparino Stefano A Serapian Francesca De Giorgi Silvia Faravelli Giorgio Colombo Federico Forneris	Multifunctional human collagen lysyl hydroxylase (LH/PLOD) enzymes catalyze post-translational hydroxylation and subsequent glycosylation of collagens, enabling their maturation and supramolecular organization in the extracellular matrix (ECM). Recently, the overexpression of LH/PLODs in the tumor microenvironment results in abnormal accumulation of these collagen post-translational modifications, which has been correlated with increased metastatic progression of a wide variety of solid tumors	pmid:36090047 pmc:PMC9453210 doi:10.3389/fmolb.2022.876352	Mon, 12 Sep 2022 06:00:00 -0400
8	pubmed:36090091	A directed genome evolution method to enhance hydrogen production in Rhodobacter capsulatus	Emma Barahona Elisa San Isidro Laura Sierra-Heras Inés Álvarez-Melcón Emilio Jiménez-Vicente José María Buesa Juan Imperial Luis M Rubio	Nitrogenase-dependent H(2) production by photosynthetic bacteria, such as Rhodobacter capsulatus, has been extensively investigated. An important limitation to increase H(2) production using genetic manipulation is the scarcity of high-throughput screening methods to detect possible overproducing mutants. Previously, we engineered R. capsulatus strains that emitted fluorescence in response to H(2) and used them to identify mutations in the nitrogenase Fe protein leading to H(2) overproduction	pmid:36090091 pmc:PMC9449697 doi:10.3389/fmicb.2022.991123	Mon, 12 Sep 2022 06:00:00 -0400
9	pubmed:36090812	YTLR: Extracting yeast transcription factor- gene associations from the literature using automated literature readers	Tzu-Hsien Yang Chung-Yu Wang Hsiu-Chun Tsai Ya-Chiao Yang Cheng-Tse Liu	Cells adapt to environmental stresses mainly via transcription reprogramming. Correct transcription control is mediated by the interactions between transcription factors (TF) and their target genes. These TF-gene associations can be probed by chromatin immunoprecipitation techniques and knockout experiments, revealing TF binding (TFB) and regulatory (TFR) evidence, respectively. Nevertheless, most evidence is still fragmentary in the literature and requires tremendous human resources to curate	pmid:36090812 pmc:PMC9449546 doi:10.1016/j.csbj.2022.08.041	Mon, 12 Sep 2022 06:00:00 -0400
10	pubmed:36091017	Plasma exosomal IRAK1 can be a potential biomarker for predicting the treatment response to renin-angiotensin system inhibitors in patients with IgA nephropathy	Jianping Wu Xiaona Wei Jiajia Li Yangang Gan Rui Zhang Qianqian Han Peifen Liang Yuchun Zeng Qiongqiong Yang	CONCLUSIONS: Plasma exosomal IRAK1 can be a potential biomarker for predicting the treatment response of RASi in patients with IgAN.	pmid:36091017 pmc:PMC9459338 doi:10.3389/fimmu.2022.978315	Mon, 12 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
11	pubmed:36091876	Chromosome 3A harbors several pleiotropic and stable drought-responsive alleles for photosynthetic efficiency selected through wheat breeding	Ahossi Patrice Koua Benedict Chijioke Oyiga Said Dadshani Salma Benaouda Mohammad Bahman Sadeqi Uwe Rascher Jens Léon Agim Ballvora	Water deficit is the most severe stress factor in crop production threatening global food security. In this study, we evaluated the genetic variation in photosynthetic traits among 200 wheat cultivars evaluated under drought and rainfed conditions. Significant genotypic, treatments, and their interaction effects were detected for chlorophyll content and chlorophyll fluorescence parameters. Drought stress reduced the effective quantum yield of photosystem II (YII) from the anthesis growth stage	pmid:36091876 pmc:PMC9440346 doi:10.1002/pld3.438	Mon, 12 Sep 2022 06:00:00 -0400
12	pubmed:36092604	Tideglusib Inhibits Pif1 Helicase of Bacteroides sp. via an Irreversible and Cys- 380-Dependent Mechanism	Xianglian Zhou Yuting Pan Yi Qu Xisong Ke	Pif1 helicase plays multiple roles in maintaining genome stability, which is an attractive therapeutic target for helicase-related diseases, while small molecules targeting Pif1 are not yet available. In this study, we performed a fluorescence polarization-based high-throughput screening and identified that an FDA-approved drug, Tideglusib (TD), could inhibit the DNA-binding activity (IC(50) = 6.2 ± 0.4 M) and ATPase and helicase activity (IC(50) = $2-4$ M) of Bacteroides sp. Pif1 (BaPif1),	pmid:36092604 pmc:PMC9453980 doi:10.1021/acsomega.2c03546	Mon, 12 Sep 2022 06:00:00 -0400
13	pubmed:36092905	Molecular basis of epigenetic regulation in cancer diagnosis and treatment	Sonam Tulsyan Mehreen Aftab Sandeep Sisodiya Asiya Khan Atul Chikara Pranay Tanwar Showket Hussain	The global cancer cases and mortality rates are increasing and demand efficient biomarkers for accurate screening, detection, diagnosis, and prognosis. Recent studies have demonstrated that variations in epigenetic mechanisms like aberrant promoter methylation, altered histone modification and mutations in ATP-dependent chromatin remodelling complexes play an important role in the development of carcinogenic events. However, the influence of other epigenetic alterations in various cancers was	pmid:36092905 pmc:PMC9449878 doi:10.3389/fgene.2022.885635	Mon, 12 Sep 2022 06:00:00 -0400
14	pubmed:36093377	TEMPOL inhibits SARS-CoV-2 replication and development of lung disease in the Syrian hamster model	Nunziata Maio Sara Cherry David C Schultz Brett L Hurst W Marston Linehan Tracey A Rouault	Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) has caused a worldwide outbreak, known as coronavirus disease 2019 (COVID-19). Alongside vaccines, antiviral therapeutics are an important part of the healthcare response to COVID-19. We previously reported that TEMPOL, a small molecule stable nitroxide, inactivated the RNA-dependent RNA polymerase (RdRp) of SARS-CoV-2 by causing the oxidative degradation of its ironsulfur cofactors. Here, we demonstrate that TEMPOL is effective in	pmid:36093377 pmc:PMC9444323 doi:10.1016/j.isci.2022.105074	Mon, 12 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
15	pubmed:36093378	The FDA-approved drug Auranofin has a dual inhibitory effect on SARS-CoV-2 entry and NF-B signaling	Emmanuel Laplantine Christine Chable-Bessia Anne Oudin Jitendryia Swain Adèle Soria Peggy Merida Manon Gourdelier Sarra Mestiri Indira Besseghe Erwan Bremaud Aymeric Neyret Sebastien Lyonnais Cyril Favard Philippe Benaroch Mathieu Hubert Olivier Schwartz Maryse Guerin Anne Danckaert Elaine Del Nery Delphine Muriaux Robert Weil	Patients with severe COVID-19 exhibit an altered immune response that fails to control viral spread and suffer from exacerbated inflammatory response, which eventually can lead to death. A major challenge is to develop an effective treatment for COVID-19. NF-B is a major player in the innate immunity and inflammatory process. By a high-throughput screening approach, we identified FDA-approved compounds that inhibit the NF-B pathway and thus dampen inflammation. Among these, we show that	pmid:36093378 pmc:PMC9439859 doi:10.1016/j.isci.2022.105066	Mon, 12 Sep 2022 06:00:00 -0400
16	pubmed:36093820	Discovery and Activity Evaluation of the Inhibitory Effect of Four Kinds Traditional Chinese Medicine Extracts on the CYP3A4 Enzyme	Chenyang Ai Xinxin Miao Lili Wang Jun He	CONCLUSION: The extracts of Abrus precatorius, Andrographis paniculata, Angelica pubescens f. biserrata and Lithospermum erythrorhizon had certain inhibitory effects on the CYP3A4 enzyme, and attention should be paid to the possible adverse reactions when they were used in combination with the CYP3A4 enzyme-substrate drugs. A combination of computational approaches might be a useful tool to identify potential inhibitors of the CYP3A4 enzyme from traditional Chinese medicine.	pmid:36093820 doi:10.2174/1386207325666220909100935	Mon, 12 Sep 2022 06:00:00 -0400
17	pubmed:36094200	Rapid Gene Target Tracking for Enhancing - Carotene Production Using Flow Cytometry- Based High-Throughput Screening in Yarrowia lipolytica	Mengmeng Liu Jin Zhang Xiaoqin Liu Jin Hou Qingsheng Qi	-Carotene is a provitamin A precursor and an important antioxidant that is used widely in the aquaculture, food, cosmetic, and pharmaceutical industries. Oleaginous Yarrowia lipolytica has been demonstrated as a competitive producer microorganism for the production of hydrophobic -carotene through rational engineering strategies. However, the limited understanding of the complexity of the metabolic network between carotenoid biosynthesis and other cellular processes has hampered further	pmid:36094200 doi:10.1128/aem.01149-22	Mon, 12 Sep 2022 06:00:00 -0400
18	pubmed:36094205	Drug Repurposing for Therapeutic Discovery against Human Metapneumovirus Infection	Annelies Van Den Bergh Patrice Guillon Mark von Itzstein Benjamin Bailly Larissa Dirr	Human metapneumovirus (HMPV) is recognized as an important cause of pneumonia in infants, in the elderly, and in immunocompromised individuals worldwide. The absence of an antiviral treatment or vaccine strategy against HMPV infection creates a high burden on the global health care system. Drug repurposing has become increasingly attractive for the treatment of emerging and endemic diseases as it requires less research and development costs than traditional drug discovery. In this study, we	pmid:36094205 doi:10.1128/aac.01008-22	Mon, 12 Sep 2022 06:00:00 -0400

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19	pubmed:36094271	Brain Ventricular Microinjections of Lipopolysaccharide into Larval Zebrafish to Assess Neuroinflammation and Neurotoxicity	Yulin He Simon Ming Yuen Lee	Neuroinflammation is a key player in various neurological disorders, including neurodegenerative diseases. Therefore, it is of great interest to research and develop alternative in vivo neuroinflammation models to understand the role of neuroinflammation in neurodegeneration. In this study, a larval zebrafish model of neuroinflammation mediated by ventricular microinjection of lipopolysaccharide (LPS) to induce an immune response and neurotoxicity was developed and validated. The transgenic	pmid:36094271 doi:10.3791/64313	Mon, 12 Sep 2022 06:00:00 -0400
20	pubmed:36094397	Universal and Sensitive Drug Assessment Biosensing Platform Using Optimal Mechanical Beating Detection of Single Cardiomyocyte	Dongxin Xu Hongbo Xiao Shuzhe Wang Hongbo Li Hui-Jiuan Chen Chuan Liu Ning Hu	The preclinical assessment of efficacy and safety is essential for cardiovascular drug development in order to guarantee effective prevention and treatment of cardiovascular disease and avoid human health endangerment and a huge waste of resources. Rhythmic mechanical beating as one of the crucial cardiomyocyte properties has been exploited to establish a drug assessment biosensing platform. However, the conventional label-free biosensing platforms are difficult to perform high-throughput and	pmid:36094397 doi:10.1021/acsnano.2c08049	Mon, 12 Sep 2022 06:00:00 -0400