high throughput screening

	NCT Number	Title	Authors	Description	Identifier	Dates
1	pubmed:35993440	Synthesis, Design, and Structure-Activity Relationship of a Benzenesulfonylpiperazine Series against Trypanosoma cruzi	Ana Clara Cassiano Martinho Daniela de Melo Resende Emanuelly Silva Landin Thibault Joseph William Jacques Dit Lapierre Talita Cristina Diniz Bernardes Luan Carvalho Martins Rafaela Salgado Ferreira Silvane Maria Fonseca Murta Celso de Oliveira Rezende Júnior	Chagas disease is a neglected tropical disease, endemic in Latin America and caused by the protozoan parasite Trypanosoma cruzi. Available treatments show low cure efficacy during the chronic phase of the disease and cause a series of side effects, reinforcing the need to develop new drugs against Chagas disease. In this work, we describe the optimization of a trypanocidal hit compound recently reported in phenotypic high-throughput screening studies against Trypanosoma cruzi. A hit-to-lead...	pmid:35993440 doi:10.1002/cmdc.202200211	Mon, 22 Aug 2022 06:00:00 -0400
2	pubmed:36067814	Use of QuEChERS as a manual and automated high-throughput protocol for investigating environmental matrices	A Ruth Godfrey Jonathan Dunscombe Anthony Gravell Ann Hunter Mark P Barrow Geertje van Keulen Claire Desbrow Rachel Townsend	Environmental pollution has strong links to adverse human health outcomes with risks of pollution through production, use, ineffective wastewater (WW) remediation, and/or leachate from landfill. 'Fit-for-purpose' monitoring approaches are critical for better pollution control and mitigation of harm, with current sample preparation methods for complex environmental matrices typically time-consuming and labour intensive, unsuitable for high-throughput screening. This study has shown that a...	pmid:36067814 doi:10.1016/j.chemosphere.2022.136313	Tue, 06 Sep 2022 06:00:00 -0400
3	pubmed:36067877	Metabolic engineering of E. coli for -alanine production using a multi-biosensor enabled approach	Shuo-Fu Yuan Priya H Nair Dominic Borbon Sarah M Coleman Po-Hsun Fan Wen-Ling Lin Hal S Alper	-alanine is an important biomolecule used in nutraceuticals, pharmaceuticals, and chemical synthesis. The relatively eco-friendly bioproduction of -alanine has recently attracted more interest than petroleum-based chemical synthesis. In this work, we developed two types of in vivo high-throughput screening platforms, wherein one was utilized to identify a novel target ribonuclease E (encoded by rne) as well as a redox-cofactor balancing module that can enhance de novo -alanine biosynthesis...	pmid:36067877 doi:10.1016/j.ymben.2022.08.012	Tue, 06 Sep 2022 06:00:00 -0400
4	pubmed:36068257	A pocket-based 3D molecule generative model fueled by experimental electron density	Lvwei Wang Rong Bai Xiaoxuan Shi Wei Zhang Yinuo Cui Xiaoman Wang Cheng Wang Haoyu Chang Yingsheng Zhang Jielong Zhou Wei Peng Wenbiao Zhou Bo Huang	We report for the first time the use of experimental electron density (ED) as training data for the generation of drug-like three-dimensional molecules based on the structure of a target protein pocket. Similar to a structural biologist building molecules based on their ED, our model functions with two main components: a generative adversarial network (GAN) to generate the ligand ED in the input pocket and an ED interpretation module for molecule generation. The model was tested on three...	pmid:36068257 doi:10.1038/s41598-022-19363-6	Tue, 06 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
5	pubmed:36068467	Pharmacogenomic Screening of Drug Candidates using Patient-Specific hiPSC-Derived Cardiomyocyte High-Throughput Calcium Imaging	Malorie Blancard K Ashley Fetterman Paul W Burridge	Calcium imaging is an invaluable technique to detect and characterize calcium flux in cells. The use of calcium dye provides information on the concentration and spatial distribution of calcium. Calcium imaging is a well-established technique to assess the calcium-induced calcium release mechanism in cardiomyocytes. It can also be used to characterize mutations in genes crucial for this mechanism that frequently causes arrhythmia. Here we describe a high-throughput methodology of calcium imaging...	pmid:36068467 doi:10.1007/978-1-0716-2573-6_10	Tue, 06 Sep 2022 06:00:00 -0400
6	pubmed:36068783	Cell models for Alzheimer's and Parkinson's disease: At the interface of biology and drug discovery	Sandra Cetin Damijan Knez Stanislav Gobec Janko Kos Anja Pišlar	Neurodegenerative diseases are severely debilitating conditions characterized primarily by progressive neuronal loss and impairment of the nervous system. Alzheimer's and Parkinson's diseases are the most common neurodegenerative disorders, and their impact is increasing as average life expectancy increases worldwide. Although the underlying mechanisms of both progressive diseases have been extensively studied, we still lack a comprehensive understanding of the molecular basis of both diseases....	pmid:36068783 doi:10.1016/j.biopha.2022.112924	Wed, 07 Sep 2022 06:00:00 -0400
7	pubmed:36069446	Fatty Acid Synthesis Knockdown Promotes Biofilm Wrinkling and Inhibits Sporulation in Bacillus subtilis	Heidi A Arjes Haiwen Gui Rachel Porter Esha Atolia Jason M Peters Carol Gross Daniel B Kearns Kerwyn Casey Huang	Many bacterial species typically live in complex three-dimensional biofilms, yet much remains unknown about differences in essential processes between nonbiofilm and biofilm lifestyles. Here, we created a CRISPR interference (CRISPRi) library of knockdown strains covering all known essential genes in the biofilm-forming Bacillus subtilis strain NCIB 3610 and investigated growth, biofilm colony wrinkling, and sporulation phenotypes of the knockdown library. First, we showed that gene essentiality...	pmid:36069446 doi:10.1128/mbio.01388-22	Wed, 07 Sep 2022 06:00:00 -0400
8	pubmed:36070142	Endocrine-Disrupting Chemicals Exposure Alter Neuroendocrine Factors, Disrupt Cardiac Functions and Provokes Hypoxia Conditions in Zebrafish Model	Sweta Thakkar Barathi Seetharaman Hamsini Kumar Ramasamy Vasantharekha	Zebrafish (Danio rerio) is an increasingly popular vertebrate model used for assessing the toxicity of endocrine-disrupting chemicals (EDCs) on living beings. The zebrafish features high genetic homology to mammals, because of its rapid embryonic development, optical transparency of phenotypic screening embryos, high throughput genetic and chemical screening which make them a powerful toxicological model. This systematic review aimed to assess the recent literature on the use of zebrafish model...	pmid:36070142 doi:10.1007/s00244-022-00955-2	Wed, 07 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
9	pubmed:36070252	SILVI, an open-source pipeline for T-cell epitope selection	Joana Pissarra Franck Dorkeld Etienne Loire Vincent Bonhomme Denis Sereno Jean-Loup Lemesre Philippe Holzmuller	High-throughput screening of available genomic data and identification of potential antigenic candidates have promoted the development of epitope-based vaccines and therapeutics. Several immunoinformatic tools are available to predict potential epitopes and other immunogenicity-related features, yet it is still challenging and time-consuming to compare and integrate results from different algorithms. We developed the R script SILVI (short for: from in silico to in vivo), to assist in the...	pmid:36070252 doi:10.1371/journal.pone.0273494	Wed, 07 Sep 2022 06:00:00 -0400
10	pubmed:36070368	Pharmacogenomic landscape of head and neck squamous cell carcinoma informs precision oncology therapy	Ziyue Gu Yanli Yao Guizhu Yang Guopei Zhu Zhen Tian Rui Wang Qi Wu Yujue Wang Yaping Wu Lan Chen Chong Wang Jiamin Gao Xindan Kang Jie Zhang Lizhen Wang Shengzhong Duan Zhongming Zhao Zhiyuan Zhang Shuyang Sun	Head and neck squamous cell carcinoma (HNSCC) is a common and frequently lethal cancer with few therapeutic options. In particular, there are few effective targeted therapies. Development of highly effective therapeutic strategies tailored to patients with HNSCC remains a pressing challenge. To address this, we present a pharmacogenomic study to facilitate precision treatments for patients with HNSCC. We established a large collection of 56 HNSCC patient-derived cells (PDCs), which recapitulated...	pmid:36070368 doi:10.1126/scitranslmed.abo5987	Wed, 07 Sep 2022 06:00:00 -0400
11	pubmed:36070569	Broad-Specificity Aptamer of Sulfonamides: Isolation and Its Application in Simultaneous Detection of Multiple Sulfonamides in Fish Sample	Ruyi Xu Chen Yang Lin Huang Wenchao Lv Weijuan Yang Yongning Wu FengFu Fu	Sulfonamide antibiotics (SAs) are widely used in animal husbandry and aquaculture, and the excess residues of SAs in animal-derived foods will harm the health of consumers. In reality, various SAs were alternately used in animal husbandry and aquaculture, and thus, it is urgent need to develop simple and high-throughput methods for simultaneously detecting multiple SAs or groups of SAs in order to realize rapid screening of total SAs residues in animal-derived foods. We herein isolated a...	pmid:36070569 doi:10.1021/acs.jafc.2c03423	Wed, 07 Sep 2022 06:00:00 -0400