high throughput screening

	NCT Number	Title	Authors	Description	Identifier	Dates
1	pubmed:36104373	Novel tricyclic small molecule inhibitors of Nicotinamide N-methyltransferase for the treatment of metabolic disorders	Sven Ruf Sridharan Rajagopal Sanjay Venkatachalapathi Kadnur Mahanandeesha S Hallur Shilpa Rani Rajendra Kristam Srinivasan Swaminathan Bharat Ravindra Zope Pavan Kumar Gondrala Indu Swamy V P Rama Kishore Putta Saravanan Kandan Gernot Zech Herman Schreuder Christine Rudolph Ralf Elvert Joerg Czech Swarnakumari Birudukota M Amir Siddiqui Niranjan Naranapura Anand Vishal Subhash Mane Sreekanth Dittakavi Juluri Suresh Ramachandraiah Gosu Mullangi Ramesh Takeshi Yura Saravanakumar Dhakshinamoorthy Aimo Kannt	Nicotinamide N-methyltransferase (NNMT) is a metabolic regulator that catalyzes the methylation of nicotinamide (Nam) using the co-factor S-adenosyl-L-methionine to form 1-methyl-nicotinamide (MNA). Overexpression of NNMT and the presence of the active metabolite MNA is associated with a number of diseases including metabolic disorders. We conducted a high-throughput screening campaign that led to the identification of a tricyclic core as a potential NNMT small molecule inhibitor series....	pmid:36104373 doi:10.1038/s41598-022-19634-2	Wed, 14 Sep 2022 06:00:00 -0400
2	pubmed:36105851	The *C. elegans* Observatory: High-throughput exploration of behavioral aging	Rex A Kerr Antoine E Roux Jérôme Goudeau Cynthia Kenyon	Organisms undergo a variety of characteristic changes as they age, suggesting a substantial commonality in the mechanistic basis of aging. Experiments in model organisms have revealed a variety of cellular systems that impact lifespan, but technical challenges have prevented a comprehensive evaluation of how these components impact the trajectory of aging, and many components likely remain undiscovered. To facilitate the deeper exploration of aging trajectories at a sufficient scale to enable...	pmid:36105851 pmc:PMC9466599 doi:10.3389/fragi.2022.932656	Thu, 15 Sep 2022 06:00:00 -0400
3	pubmed:36106408	Combinatorial screening SlipChip for rapid phenotypic antimicrobial susceptibility testing	Xiang Li Xu Liu Ziqing Yu Yang Luo Qixin Hu Zhenye Xu Jia Dai Nannan Wu Feng Shen	Antimicrobial resistance (AMR) by bacteria is a serious global threat, and a rapid, high-throughput, and easy-to-use phenotypic antimicrobial susceptibility testing (AST) method is essential for making timely treatment decisions and controlling the spread of antibiotic resistant micro-organisms. Traditional culture-based methods are time-consuming, and their capability to screen against a large number of different conditions is limited; meanwhile genotypic based methods, including sequencing and...	pmid:36106408 doi:10.1039/d2lc00661h	Thu, 15 Sep 2022 06:00:00 -0400

	NCT Number	Title	Authors	Description	Identifier	Dates
4	pubmed:36106953	Identification of novel inhibitors of *Neisseria gonorrhoeae* MurI using homology modeling, structure-based pharmacophore, molecular docking, and molecular dynamics simulation-based approach	Ravi Kant Prakash Jha Daman Saluja Madhu Chopra	MurI is one of the most significant role players in the biosynthesis of the peptidoglycan layer in Neisseria gonorrhoeae (Ng). We attempted to highlight the structural and functional relationship between Ng-MurI and D-glutamate to design novel molecules targeting this interaction. The three-dimensional (3D) model of the protein was constructed by homology modeling and the quality and consistency of generated model were assessed. The binding site of the protein was identified by molecular docking...	pmid:36106953 doi:10.1080/07391102.2022.2121943	Thu, 15 Sep 2022 06:00:00 -0400
5	pubmed:36107631	Modeling pesticide residue uptake by leguminous plants: A geocarpic fruit model for peanuts	Zijian Li	CONCLUSIONS: The simulation results have some degrees of agreement with field measurements, indicating that the proposed model can be used as a screening tool for dietary risk assessment of pesticides in peanuts. In future research, pH-dependent physicochemical properties (e.g., soil-water partition coefficient and TSCF) and degradation rate constants of chemicals need to be refined to improve the simulation analysis. This article is protected by copyright. All rights reserved.	pmid:36107631 doi:10.1002/ps.7184	Thu, 15 Sep 2022 06:00:00 -0400
6	pubmed:36107744	Scalable CRISPR-Cas9 chemical genetic screens in non-transformed human cells	Kevin Lin Ya-Chu Chang Ezequiel Marron Fernandez de Velasco Kevin Wickman Chad L Myers Anja-Katrin Bielinsky	Pooled lentiviral CRISPR-Cas9 screens are utilized for assessing the differential sensitivity or resistance of many single-gene knockouts to a compound. Here, we present a scalable approach for high-throughput compound screening by utilizing a small custom library. We describe steps to perform a proof-of-principle chemical screen in non-transformed hTERT RPE-1 TP53^(-/-) cells with higher coverage and greater timepoint resolution compared to genome-wide screens. This approach can be adapted for...	pmid:36107744 doi:10.1016/j.xpro.2022.101675	Thu, 15 Sep 2022 06:00:00 -0400
7	pubmed:36107884	Highly multiplexed selection of RNA aptamers against a small molecule library	Brent Townshend Matias Kaplan Christina D Smolke	Applications of synthetic biology spanning human health, industrial bioproduction, and ecosystem monitoring often require small molecule sensing capabilities, typically in the form of genetically encoded small molecule biosensors. Critical to the deployment of greater numbers of these systems are methods that support the rapid development of such biosensors against a broad range of small molecule targets. Here, we use a previously developed method for selection of RNA biosensors against...	pmid:36107884 doi:10.1371/journal.pone.0273381	Thu, 15 Sep 2022 06:00:00 -0400
8	pubmed:36108302	The National Laboratory Response to the COVID-19 Pandemic in Taiwan	Ji-Rong Yang Hwa-Jen Teng Jou-Han Chen Hsin-I Huang Ming-Tsan Liu Shu-Ying Li	From April 23 to November 2021, a wave of COVID-19 infections caused by a new Alpha variant swept across Taiwan, resulting in 14,458 positive cases and 830 deaths among over 3.8 million people tested. To cope with the sudden increase in sample volume, as of December 14, 2021, a network of 249 laboratories with a total diagnostic capacity of 158,492 real-time reverse transcription polymerase chain reaction tests per day was established in 22 administrative regions. As of April 2022, over 9.5...	pmid:36108302 doi:10.1089/hs.2022.0024	Thu, 15 Sep 2022 06:00:00 -0400