

high throughput screening

NCT Number		Title	Authors	Description	Identifier	Dates
1	pubmed:36122548	High throughput virtual screening (HTVS) of peptide library: Technological advancement in ligand discovery	Nitesh Mani Tripathi Anupam Bandyopadhyay	High-throughput virtual screening (HTVS) is a leading biopharmaceutical technology that employs computational algorithms to uncover biologically active compounds from large-scale collections of chemical compound libraries. In addition, this method often leverages the precedence of screening focused libraries for assessing their binding affinities and improving physicochemical properties. Usually, developing a drug sometimes takes ages, and lessons are learnt from FDA-approved drugs. This...	pmid:36122548 doi:10.1016/j.ejmech.2022.114766	Mon, 19 Sep 2022 06:00:00 -0400
2	pubmed:36125104	Discovery of potential hypoglycemic metabolites in Cassiae Semen by coupling UHPLC-QTOF-MS/MS combined plant metabolomics and spectrum-effect relationship analyses	Fei Yang Yanfang Zou Chenyue Li Jiaxu Li Yaping Zang Xin Peng Juan Wang E-Hu Liu Shengqiang Tong Chu Chu	Cassiae Semen (CS) is consumed as fried tea or medicinal food in Asian areas. Its two commercial forms, namely raw and fried CS, exert different clinical applications, in which fried CS is commonly applied as a functional tea for losing weight. To prevent confusion in the use of the two forms of CS, a comprehensive strategy by combining plant metabolomics and spectrum-effect relationship analyses was developed for the fast and efficient discrimination of raw and fried CS, and further for the...	pmid:36125104 doi:10.1039/d2fo00562j	Tue, 20 Sep 2022 06:00:00 -0400
3	pubmed:36125920	Rapid Quantitation of Anatoxins in Benthic Cyanobacterial Mats Using Direct Analysis in Real-Time-High-Resolution Tandem Mass Spectrometry	Daniel G Beach Meghann Bruce Janice Lawrence Pearse McCarron	Toxic benthic cyanobacterial mats are increasingly reported worldwide as being responsible for animal mortalities due to their production of the potent neurotoxin anatoxin-a (ATX) and its analogues. Improved analytical methods for anatoxins are needed to address public health and watershed management challenges arising from extremely high spatial and temporal variability within impacted systems. We present the development, validation, and application of a direct analysis in...	pmid:36125920 doi:10.1021/acs.est.2c05426	Tue, 20 Sep 2022 06:00:00 -0400

NCT Number		Title	Authors	Description	Identifier	Dates
4	pubmed:36126059	Identification of RP-6685, an Orally Bioavailable Compound that Inhibits the DNA Polymerase Activity of Pol	Monica Bubenik Pavel Mader Philippe Mochirian Frédéric Vallée Jillian Clark Jean-François Truchon Alexander L Perryman Victor Pau Igor Kurinov Karl E Zahn Marie-Eve Leclaire Robert Papp Marie-Claude Mathieu Martine Hamel Nicole M Duffy Claude Godbout Matias Casas-Selves Jean-Pierre Falguyret Prasamit S Baruah Olivier Nicolas Rino Stocco Hugo Poirier Giovanni Martino Alexanne Bonneau Fortin Anne Roulston Amandine Chefson Stéphane Dorich Miguel St-Onge Purvish Patel Charles Pellerin Stéphane Ciblat Thomas Pinter Francis Barabé Majida El Bakkouri Paranjay Parikh Christian Gervais Agnel Sfeir Yael Mamane Stephen J Morris W Cameron Black Frank Sicheri Michel Gallant	DNA polymerase theta (Pol) is an attractive synthetic lethal target for drug discovery, predicted to be efficacious against breast and ovarian cancers harboring BRCA-mutant alleles. Here, we describe our hit-to-lead efforts in search of a selective inhibitor of human Pol (encoded by POLQ). A high-throughput screening campaign of 350,000 compounds identified an 11 micromolar hit, giving rise to the N2-substituted fused pyrazolo series, which was validated by biophysical methods. Structure-based...	pmid:36126059 doi:10.1021/acs.jmedchem.2c00998	Tue, 20 Sep 2022 06:00:00 -0400
5	pubmed:36126276	Plasma miR-151-3p as a candidate diagnostic biomarker for head and neck cancer: a cross-sectional study within the INHANCE consortium	Roberta Pastorino Michele Sassano Danilo Francesco Tiziano Luca Giraldi Rosarita Amore Dario Arzani Emanuela Abiusi Wolfgang Ahrens Laia Alemany Vilches Cristina Canova Claire Mary Healy Ivana Holcatova Pagona Lagiou Jerry Polesel Maja Popovic Ståle Nygård Gabriella Cadoni Ariana Znaor Paolo Boffetta Keitaro Matsuo Isao Oze Paul Brennan Stefania Boccia	CONCLUSIONS: We identified miR-151-3p as an early marker of HNC. This miRNA was the only upregulated in patients at early stages of the disease, independently of the smoking status.	pmid:36126276 doi:10.1158/1055-9965.EPI-22-0376	Tue, 20 Sep 2022 06:00:00 -0400