

Poster Presentation September 2th,2019			
Submission	Title	track	Poster number
106846	Predictions of the interaction between Triazaspiro and BACE1 enzyme	SDD	SDD01
107647	Synthesis of new analogues of marinoquinolines and their biological activity against malaria	SDD	SDD02
111532	Computationally guided drug repositioning: QSAR-based Virtual Screening of Macrolides for Schistosomiasis	SDD	SDD03
108950	Molecular Dynamics Simulations of Arthropods Antimicrobial Peptides Css54 and La47 with POPC and POPG membranes	SDD	SDD04
108955	Molecular docking: guidelines to a low-cost methodology	SDD	SDD05
108962	Discovery of hit compounds against Paracoccidioides spp. through similarity search	SDD	SDD06
108968	Rational design of peptides against glyceraldehyde-3-phosphate dehydrogenase as potential candidates for the treatment of paracoccidioidomycosis	SDD	SDD07
108969	Design of inhibitor peptides to modulate isocitrate lyase interactions in Paracoccidioides lutzii	SDD	SDD08
108970	Methylcitrate synthase inhibitors from Paracoccidioides lutzii: a approach by virtual screening and antifungal activity	SDD	SDD09
108972	Rescuing poorly soluble drugs: a cheminformatics approach for polymeric micelle-drug formulations	SDD	SDD10
108975	Discovering drug repurposing opportunities for the treatment of Chagas disease using ligand-based machine learning methods	SDD	SDD11
108981	Expanding the universe of membranolytic AMPs	SDD	SDD12
108998	Targeting 20s proteasome with computational tools	SDD	SDD13
109000	Molecular Architect (MolAr): A Structure Based Virtual Screening software	SDD	SDD14
111551	Machine Learning models for virtual screening of new schistosomicidal compounds	SDD	SDD15
109003	Quantitative Structure-Activity Relationship Models for Cryptococcosis: A Virtual Screening Approach	SDD	SDD16
109006	Structural optimization of Schistosoma mansoni aspartyl protease inhibitors: integration of computational and experimental methods	SDD	SDD17

109009	Identification of multi-target compounds against Alzheimer's disease	SDD	SDD18
109010	Fragment-based discovery of Schistosoma mansoni Thioredoxin Glutathione Reductase (SmTGR) inhibitors: Second generation of structurally optimized leads identified by X-ray crystallography	SDD	SDD19
109012	Search for inhibitors against PfPMT by Ligand and Structure Virtual Screening	SDD	SDD20
109022	Identification of ligand binding hot spots on Leishmania chagasi superoxide dismutase by ligand competitive saturation	SDD	SDD21
109031	Dynamic Behavior of Dengue and Zika viruses NS1 protein reveals monomer-monomer interaction mechanisms and insights to rational drug design	SDD	SDD22
111697	Machine Learning models for prediction of acute dermal toxicity	SDD	SDD23
109034	In silico planning of coumarins as possible inhibitors of Kinesin Eg5	SDD	SDD24
109042	Bioactive compounds design pharmacophore-based with antibacterial activity in MRSA strains	SDD	SDD25
109044	In silico chemogenomics repositioning strategy identifies a novel candidate for malaria treatment	SDD	SDD26
109138	Improving the prediction of binding site and pose of allosteric modulators of GSK-3 β related to Alzheimer's disease	SDD	SDD27
109165	Evaluation of docking methodologies for DNA-ligand systems	SDD	SDD28
109193	Coupling Yeast Surrogate Genetics with In Silico Modelling and Virtual Ligand Screening for Target-based Drug Discovery: the neglected vivax malaria case	SDD	SDD29
109205	In silico study in the drug design for essential tremor treatment	SDD	SDD30
111469	STopTox: A machine learning app as an alternative to animal testing for acute systemic and topical toxicity	SDD	SDD31
110317	Targeting Rpf-interacting protein A (RipA) from M. tuberculosis using a fragment-based drug design approach	SDD	SDD32
110324	Aminoacyl-tRNA synthetases: A new molecular target against Chagas Disease by Drug Repurposing	SDD	SDD33

111520	Development and validation of QSAR-based machine learning models for screening of DPP-IV inhibitors	SDD	SDD34
110328	In silico and In vitro investigation of cruzain and rhodesain inhibitors in the Pathogen Box	SDD	SDD35
110342	Ligand-based Pharmacophore Modeling for Discovery of Potential 14- α -demethylase Inhibitors.	SDD	SDD36
110353	Inclusion of Receptor Flexibility in the DockThor Program through the Soft Docking Approach	SDD	SDD37
110371	Molecular dynamics simulations of the amyloid- β peptide in aqueous solution of the cucurbit[7]uril	SDD	SDD38
111104	Integrative Similarity analysis, Docking and Machine Learning models for identifying new Zika NS5 hits guided by Dengue NS5 inhibitors	SDD	SDD39
115619	Identification Of Brazilian Biodiversity Products And Approved Drugs As Potential Anti-Inflammatory Agents, Irak-1 And Irak-4 Inhibitors	SDD	SDD40
105076	Heterocyclic medicinal chemistry: development of innovative fragment library	MCSC	MCSC01
107430	Novel 8-hydroxyquinoline derivatives are potential candidates for treatment of fungal infections: toxicity, irritability and PK/PD modeling studies	MCSC	MCSC02
107836	Planning, Synthesis And Biological Evaluation Of New Analogs To Zidovudin, Amprenavir And Tenofovir	MCSC	MCSC03
107980	Design, synthesis and biological of new potential reverse transcriptase inhibitors containing acyclic phosphonate	MCSC	MCSC04
108002	Pteridine scaffold as candidate for MRCK γ kinase inhibitor	MCSC	MCSC05
108217	Studies on the synthesis of novel tacrine-tiazole hybrids as potential acetylcholinesterase reactivators	MCSC	MCSC06
108854	Lead-Optimization of 1-(4-aryl)cyclohexyl-4-(3-pyridyl)piperazine as TRPV6 Inhibitors	MCSC	MCSC07
108856	Evaluation of the Antihistamines LINS01 as Ligands of the Dopamine D2/D3 Receptors	MCSC	MCSC08
108860	Synthesis and biological evaluation of cysteine protease inhibitors	MCSC	MCSC09
108875	PH157 is a promising candidate to treat fungal infections associated with biofilm formation	MCSC	MCSC10

108876	Multiple Synthetic Strategies For The Generation Of Triazolylpeptidyl Penicillin Analogs In The Search For New Antitumoral Compounds	MCSC	MCSC11
108878	Aza indolizidines – synthesis and biological evaluation as glycosidase inhibitors	MCSC	MCSC12
108908	Synthesis of a chiral building block to obtain a cruzain inhibitor	MCSC	MCSC13
108917	Synthesis of pyrazinyl derivatives containing a benzylpiperazine moiety with potential activity against tuberculosis	MCSC	MCSC14
108920	Screening of LINS05 compounds as acetylcholinesterase inhibitors	MCSC	MCSC15
108947	Synthesis and antitrypanosomal activitie of coumarinic N-acylhydrazonic derivatives	MCSC	MCSC16
108960	Marinoquinolines As Anticancer Agents: Discovery Of New Highly Active And Selective Derivatives	MCSC	MCSC17
108963	LINS01 Compounds as Vasodilating Agents: Investigation of Potency on an Aortic Ring Ex Vivo Model	MCSC	MCSC18
108965	First-time Assessment of Camphor hydrazone derivatives as an agent against Leishmania amazonensis	MCSC	MCSC19
108967	Antitrypanosomal aminobenzimidazoles: hit to lead expansion of new chemical entities against Trypanosoma cruzi and Leishmania infantum	MCSC	MCSC20
108974	Exploring pyridine-based ligands against human vaccinia-related kinases 1 and 2	MCSC	MCSC21
108976	Synthesis and study of L-cysteine-arylamides as potential protease inhibitors	MCSC	MCSC22
108977	Anti-Trypanosomal Activity of Cyclic Amine-Chalcone Hybrids	MCSC	MCSC23
108984	Synthesis of new derivatives of imatinib with antimyeloproliferative activity	MCSC	MCSC24
108987	New derivatives of imatinib with antimyeloproliferative activity	MCSC	MCSC25
108989	Imatinib and bosutinib new analogues as potentials anti-myeloproliferative agents	MCSC	MCSC26
108990	New etravirine analogues as potential inhibitors of HIV-1 reverse transcriptase and Mycobacterium tuberculosis	MCSC	MCSC27

108991	New isatin derivatives, analogues of efavirenz, as HIV-1 inhibitors	MCSC	MCSC28
108992	Carbamoylimidazoles as Potent Cruzain Inhibitors with in Vitro and in Vivo Trypanocidal Activity: a Structure-Based Drug Design Approach	MCSC	MCSC29
108993	Efforts towards a STK10/LOK chemical probe	MCSC	MCSC30
108994	Synthesis and characterization of potential pro-resolving inflammation compounds	MCSC	MCSC31
108995	Development and characterization of functionalized silica nanoparticles containing doxorubicin: a study of the influence of functionalization on the cellular aspects of cancer	MCSC	MCSC32
108996	Structural design and molecular modeling of Copper (II) complexes as inhibitors of human Topoisomerase II α .	MCSC	MCSC33
108997	Docking Analysis of LINS01 Compounds Binding at Histamine H3 and H4 Receptors Led to Novel Improved Compounds	MCSC	MCSC34
108999	Study of the cytotoxicity and mechanism of action of the new homologues of LASSBio-1586.	MCSC	MCSC35
109004	Design, synthesis and biological evaluation of new analogues of imatinib	MCSC	MCSC36
109013	Design, computational studies and synthesis of sulfonamide derivatives targeting DAGL- α enzyme for the treatment of obesity	MCSC	MCSC37
109016	Capsaicin-like analogue induced selective apoptosis in A2058 melanoma cells: Design, synthesis and molecular modeling	MCSC	MCSC38
109017	In vitro and in silico screening of chalcones against urease	MCSC	MCSC39
109021	Docking and Pharmacokinetic studies on derivatives diaryl sulfide conjugated to mepacrine against Trypanosoma cruzi Trypanothione Reductase	MCSC	MCSC40
109023	Marinoquinolines as highly active and selective antimalarial compounds	MCSC	MCSC41
109024	Synthesis and evaluation of antileukemic activity of 2-carbomethoxy-3- substituted indoles	MCSC	MCSC42
109025	Vanillin-related N-acylhydrazones: Synthesis, antischistosomal properties and target fishing studies	MCSC	MCSC43
109026	Michael addition reaction of reduced glutathione to halogenated bischalcones	MCSC	MCSC44

109027	Synthesis and study of anti-inflammatory activity of amides derived from NSAIDs and their derived S-Nitrosothiols.	MCSC	MCSC45
109029	Structure-activity relationships of sulfonamides derived from carvacrol as new agents for the treatment of Alzheimer's disease	MCSC	MCSC46
109033	Efforts towards macrocyclic dihydrofolate reductase inhibitors	MCSC	MCSC47
104268	Chalcones – Prosperous candidates for drug development	MCNP	MCNP01
107204	Cheminformatic Analysis of Natural Products	MCNP	MCNP02
111077	Discovery of new Zika virus candidates: natural products from <i>Angelica keiskei</i> with activity against NS2B-NS3 protease	MCNP	MCNP03
108982	Chemical fingerprint by LC-HRMS investigating extracts of <i>Qualea grandiflora</i> Mart. with antiplasmodial activity	MCNP	MCNP04
109028	Investigation of Cholinesterase Inhibition of New Cassine/Spectraline Analogues	MCNP	MCNP05
109326	<i>Cecropia hololeuca</i> protease inhibitors reduced nitric oxide in RAW264.7 and J774A.1 macrophages	MCNP	MCNP06
109328	Alcoholic Extract of <i>Anadenanthera colubrina</i> Improves Inflammatory Mediators In Vitro and In Vivo Paw Edema	MCNP	MCNP07
111212	Discovery of flavonoids from <i>Pterogyne nitens</i> with potent activity against Zika virus protease and helicase	MCNP	MCNP08
110377	Prediction of the biological activity and kefirin docking study	MCNP	MCNP09
110399	Evaluation of antioxidant potential and DNA damage in aqueous extract of <i>Luehea divaricata</i> leaves.	MCNP	MCNP10

Poster Presentation September 4th, 2019

Submission	Title	track	Poster number
110359	QSAR-Based Virtual Screening of Potential Anti-Candida Hit Compounds	SDD	SDD41
110380	Modified ethanalamides as unprecedented inhibitors of the <i>Chromobacterium violaceum</i> Quorum Sensing.	SDD	SDD42

110381	DockThor-VS: A Free Docking Server For Protein-Ligand Virtual Screening using the Supercomputer SDumont	SDD	SDD43
110395	Technological prospecting for neuropathic pain: monitoring the technological horizon of biopharmaceuticals	SDD	SDD44
110414	Structure Optimization of Bioactive Peptides	SDD	SDD45
110433	Quantum analysis on the PI3K/AKT/mTOR-NF- κ B pathway inhibition on DLBCL treatment	SDD	SDD46
110435	Molecular dynamics studies of G protein-coupled Adenosine A2B receptor	SDD	SDD47
110523	Analysis of physicochemical properties of bioactive molecules on dopaminergic D1 receptors to be used in the treatment of chemical dependence on cocaine	SDD	SDD48
109014	3D QSAR Studies for a Series of Trypanosoma cruzi Dihydroorotate Dehydrogenase Inhibitors	SDD	SDD49
110549	Prediction of biological activity on the cannabinoid receptor CB1 of compounds as prototypes of drugs candidates for the treatment of Cannabis sativa withdrawal syndrome	SDD	SDD50
114179	Structural biology and ligand search for the NS5 protein of the Zika virus	SDD	SDD51
109261	Plasmodium NEK-1 kinase Protein: Potential targets for disease control	SDD	SDD52
116071	Integrative Multi-kinase Approach for the Identification of Potent Antiplasmodial Hits	SDD	SDD53
108915	Development of new potential Mycobacterium tuberculosis enoyl-ACP reductase inhibitors	SDD	SDD54
109001	Artificial intelligence-driven research for drug discovery: tackling Chagas disease	SDD	SDD55
111557	Ensemble docking model for the identification of PI3K δ ligand	SDD	SDD56
111636	New insights into designing nanoparticle-mediated delivery for central nervous system diseases: Signaling and gene regulatory networks in epidermal growth factor	SDD	SDD57
111656	Hotspot guided evaluation of docked poses	SDD	SDD58
111679	ChemFlow: Standardized Workflows for Computational Chemistry	SDD	SDD59

109032	Structure-activity relationships of new Schiff bases derived from diaminomaleonitrile as new agents for the treatment of Chagas disease	SDD	SDD60
111729	Fumbling through cryptic sites: a nsP2 Chikungunya Drug discovery case study	SDD	SDD61
111732	Virtual screening and experimental validation of inhibitors of Plasmodium spp. casein kinases, CK1 and CK2 α , as potential antimalarial candidates	SDD	SDD62
111757	The InsilicAll Platform: Drug Discovery through Artificial Intelligence and Big Data	SDD	SDD63
111851	Molecular Docking of Thiosemicarbazones as Candidate Inhibitors of a Dengue-Associated Metalloprotease	SDD	SDD64
111874	Machine Learning models for prioritizing the synthesis of xanthone derivatives as promising antibacterial agents against methicillin-resistant Staphylococcus aureus	SDD	SDD65
111923	Car-Parrinello Molecular Dynamics study of the glucosamine complexation with calcium ion	SDD	SDD66
111942	A multi-parametric optimization approach in the lead identification and lead optimization stages of drug discovery	SDD	SDD67
111929	Integrative Target Prediction, Molecular docking and Experimental Evaluation of the Antidepressant-like effects of Doxycycline	SDD	SDD68
111974	Sulfonylhydrazones as novel antimalarial scaffold: design, synthesis, biological evaluation and machine learning models for structure-activity relationship interpretation	SDD	SDD69
111991	Efficient Identification of Novel Anti-Glioma Lead Compounds by Machine Learning Models	SDD	SDD70
112276	The Next Era of Pharmaceutical Research: From Bayesian Models to Deep Learning	SDD	SDD71
112680	Antiviral candidates discovery based on the structure of the yellow fever NS5 RNA-dependent RNA polymerase enzyme.	SDD	SDD72
112704	Fragment screening against Schistosoma mansoni dihydroorotate dehydrogenase: a modern approach for drug discovery	SDD	SDD73
114124	Unravelling nitroreductase function in Trypanosoma cruzi	SDD	SDD74

114135	Characterization of the dimer interface role in the Trypanosoma cruzi fumarate hydratase catalytic mechanism	SDD	SDD75
114136	Schistosoma mansoni class II fumarase: first steps for validation as drug target	SDD	SDD76
114028	Molecular modeling and cytotoxic activity of a novel bischalcone	SDD	SDD77
114165	Structural Studies of the NS2B-NS3 Protease Complex of the Brazilian Circulating Strain of Yellow Fever Virus	SDD	SDD78
109037	Structure-activity relationships of β -chalcogenamines: synthesis, enzyme inhibition, molecular docking and QSAR studies	MCSC	MCSC48
109039	Hidroxymethylnitrofurazone (NFOH) in experimental Trypanosoma cruzi infections is more efficient and decrease damage in the chronic stage than acute stage	MCSC	MCSC49
109064	Structure-based design and synthesis of new benzothiophene derivatives as potent PRPF4 kinase inhibitors	MCSC	MCSC50
109168	Development of new glutaminase inhibitors with potential antitumor action	MCSC	MCSC51
109249	Design, synthesis, in silico prediction of ADMETox properties and antineoplastic evaluation of alpha-aryltetralones and alpha-fluoro-alpha-aryltetralones derivatives	MCSC	MCSC52
109269	Leishmanicidal Activity, Cytotoxicity and Electrochemical Investigation of LQB nitrones	MCSC	MCSC53
110275	Furoxans and tocopherol analogs–furoxan hybrids as anticancer agents	MCSC	MCSC54
110276	New lipophilic derivatives of isoniazid for screening of their antimycobacterial activity	MCSC	MCSC55
110282	Determination of the 3D structure of a new tetraketone tyrosinase activator using Nuclear Magnetic Resonance	MCSC	MCSC56
110286	An Open Science, Medicinal Chemistry Program to Develop New Therapeutics Against Non-Tuberculous Mycobacteria	MCSC	MCSC57
110322	Chemosensitizer effect of cisplatin-treated bladder cancer cells by phenazine-5,10-dioxide derivatives.	MCSC	MCSC58
110335	Synthesis of substituted isoxazoles as building blocks for the synthesis of bioactive molecules	MCSC	MCSC59

110379	Disubstituted coumarins as potential inhibitors of the <i>Chromobacterium violaceum</i> Quorum Sensing	MCSC	MCSC60
110382	Antiepileptic properties of new selenobenzimidazole derivatives: a preclinical study in neonatal model of epilepsy	MCSC	MCSC61
110426	Nitroheterocyclic N-acylhydrazones as antischistosomal agents	MCSC	MCSC62
110431	Evaluation of Cholinesterase Inhibitors for Alzheimer's Disease	MCSC	MCSC63
110432	Latentiation as a strategy to design derivatives of a trypanocidal isoxazole compound	MCSC	MCSC64
109036	Design and Obtaining of Novel Naphthoquinones Hybrids	MCSC	MCSC65
111502	Sulfated derivatives of sugars: sweet spots on the modulation of the antiviral activity	MCSC	MCSC66
111686	Synthesis And Evaluation Of New Piperonyl-Cinnamoyl Hybrid Compounds With Leishmanicidal Activity	MCSC	MCSC67
111698	Design, Synthesis and Evaluation of 3-thio-1,2,4-triazoles as a Novel Class of Glutaminase Inhibitors	MCSC	MCSC68
111689	Synthesis and Evaluation of Mycobacterial ClpP1P2 Inhibitors	MCSC	MCSC69
111811	Metabolic stability of LASSBio-1632 in rat liver microsome	MCSC	MCSC70
111863	Design, synthesis and SAR evaluation of chalcones against sensitive and multidrug-resistant <i>Mycobacterium tuberculosis</i>	MCSC	MCSC71
111865	Synthesis and biological evaluation of bis-chalcones against <i>Trypanosoma cruzi</i>	MCSC	MCSC72
111881	Design, Synthesis and Anti- <i>Trichomonas vaginalis</i> Activity of Hydroxychalcones	MCSC	MCSC73
111885	4'-hydroxychalcones antibacterial activity: a combination between membrane and divisional septum disruptions	MCSC	MCSC74
111886	Antitumoral Activity of Coumarin Derivatives Synthesized by Suzuki-Miyaura Reaction	MCSC	MCSC75
111888	Methoxychalcones: Antimicrobial and Antiproliferative Activities	MCSC	MCSC76
111905	Hybridization Approach for Drug Design in Anti-leishmanial Cinnamoylhydrazones	MCSC	MCSC77

111906	Synthesis and docking study for compounds analogs of LSD1 inhibitor.	MCSC	MCSC78
112115	Repurposing the antipsychotic drug chlorpromazine for the inhibition of urinary catheter-associated biofilms	MCSC	MCSC79
112355	Design, synthesis and evaluation of novel thalidomide-donepezil hybrids as new inhibitors of AChE for the treatment of Alzheimer's disease	MCSC	MCSC80
112483	CNN1 inhibits topoisomerase I in preclinical models of chronic myeloid leukemia (CML)	MCSC	MCSC81
112514	Indole-based Compounds are Endowed with Efficient Activity Against Mycobacterium tuberculosis	MCSC	MCSC82
112665	Antiprionic activity of 6-aminoquinolones and their dimeric banzoquinone conjugates	MCSC	MCSC83
112675	Design, Synthesis and Anti-Trypanosomal Activity of Novel Nitrofurans Isoxazole Analogues of Nifurtimox	MCSC	MCSC84
112678	Synthesis and Pharmacological Evaluation of 1,5-diaryl-3-amine-1,2,4-triazoles Designed as Cholinesterase Inhibitors for the Treatment of Alzheimer's Disease	MCSC	MCSC85
112684	Analysis of the bactericidal activity of 2-amino-5,6,7,8-tetrahydro- 7,7-dimethyl-5-oxo-4-phenyl-4H-chromene-3-carbonitrile	MCSC	MCSC86
112686	Synthesis, antimicrobial evaluation and structure-activity relationship of Hexahydroimidazo [1,2- α] pyridines derivatives	MCSC	MCSC87
112705	Coumarin-benzimidazole hybrids: synthesis, antioxidant potential and biological evaluation against antimicrobial agent	MCSC	MCSC88
114141	Discovery of 1,2,4-oxadiazole derivatives as a novel class of inhibitors of 3-hydroxykynurenine transaminase (HKT) from Aedes aegypti	MCSC	MCSC89
114190	Porphyryns and Breast Cancer Resistance (ABCG2): turning substrates in a new class of inhibitors	MCSC	MCSC90
114191	Carbazoles derivatives: a brand-new class of potent, specific and non-cytotoxic ABCG2 inhibitors	MCSC	MCSC91
114192	Design, synthesis and biological evaluation of potential antitumor agents analogues from sanguinarine	MCSC	MCSC92
114194	Evaluation of Nitroheterocyclics compounds against intracellular amastigotes of Leishmania infantum	MCSC	MCSC93

114483	Aryl Benzimidazoles: A new lead in malaria drug discovery	MCSC	MCSC94
115303	Structure-Based Design, Synthesis and Pharmacological Evaluation of hydrazide derivatives as Myeloperoxidase Inhibitors	MCSC	MCSC95
110405	Pharmacokinetic and Toxicological Properties of Kefiran	MCNP	MCNP11
110421	Molecular Modeling Of Methylxanthines And Tannins For The Treatment Of Alzheimer's disease	MCNP	MCNP12
110436	Evaluation Of The Anti-Inflammatory Activity Of Aspergillus Fischeri	MCNP	MCNP13
108866	Effect of the Meta Substitution on LINS03 Analogues - Antitrypanosoma Activity and Selectivity	MCNP	MCNP14
110369	Semisynthesis of O-glycosylated derivatives of O-methyl-olivitol, isolated from Eugenia catharinae O. Berg.	MCNP	MCNP15
111624	Screening of cerrado plants against urease from Canavalia gladiata	MCNP	MCNP16
111668	Computational approaches for discovery of alkaloids with schistosomicidal activity	MCNP	MCNP17
110354	Lipinski's Ro5 and Veber rules: an analysis of the natural-product-based molecules active against Trypanosoma cruzi	MCNP	MCNP18
111951	Dereplication of extracts and DNA fingerprinting of potentially antimalarial species of the Psychotria genus (Rubiaceae)	MCNP	MCNP19
112657	Marine-derived chromomycin A5: a novel strategy to treat TBX2-driven cancers	MCNP	MCNP20
115678	Antioxidant and antileishmanial studies of phytochelators as potential candidates for optimization	MCNP	MCNP21