



# 2017 CHPC National Conference

## Monday 04 December 2017

### Chemistry: I Chemistry & Health - Satre (11:00-12:30)

-Conveners: Andre Stander

time	[id] title	presenter
11:00	[14] Computational Modeling to support the development of biosensing devices	Prof. BISETTY, Krishna
11:30	[100] Exploring chemical space using in silico studies to identify novel inhibitors of Acetylcholinesterase, a target for Alzheimer's disease	Mr VAN DER WESTHUIZEN, Carl Johan
11:50	[97] Probing the catalytic mechanism of an antifibrotic copper metallodrug	Ms LUBBE, Lizelle
12:10	[21] Lead optimization: calculating relative binding free energies with FEP+	Dr EHRLICH, Stephan

## Tuesday 05 December 2017

### Chemistry: II Chemistry & Health - Martells (11:00-12:30)

**-Conveners: Gert Kruger**

time	[id] title	presenter
11:00	[60] Molecular modelling of ligands, receptors and enzymes for in silico drug discovery	Prof. PILLAY, Tahir
11:30	[74] Using docking and molecular dynamics to design potent and selective anticancer, anti-osteoclastogenic and anti-malarial compounds	Dr STANDER, Andre
11:50	[140] The identification of highly potent peptide scaffolds for the treatment of hormone resistant prostate cancer	Mr SIGAUKE, Lester
12:10	[89] The enzymatic mechanism of Human Immunodeficiency Virus type 1 (HIV-1) protease: are we there yet?	Ms LAWAL, Monsurat Motunrayo

### Chemistry: III - Martells (13:30-15:00)

**-Conveners: Ignacy Cukrowski**

time	[id] title	presenter
13:30	[46] Computational chemistry methods in understanding the properties of porous material	Prof. ESTERHUYSEN, Catharine
14:00	[130] Can we reach the heaven of chemical accuracy by climbing Jacob's Ladder? A DFT validation study for Non-heme Iron complexes	Dr ADEYINKA, Adedapo
14:20	[99] Molecular modelling of lanthanide(III) chloride complexes with the nitrogen ligand DPA: AIM/NCI analysis and ligand conformational search	Mr MATTHEWS, Cameron
14:40	[24] A DFT study of the ring opening mechanism of tetraethyl-2-aryl-1,2-epoxygembisphosphonates	Dr SINGH, Thishana

# Wednesday 06 December 2017

## Chemistry: Chemistry - Martells (13:30-15:00)

-Conveners: Catharine Esterhuysen

time	[id] title	presenter
13:30	[186] DFT for isomers in solution, redox potentials, transition states and favored reaction products	Prof. VON ESCHWEGE, Karel
13:50	[174] FAMSEC-based insight on the chemical nature of the XH...HY (X,Y = C,N) intramolecular interactions	Prof. CUKROWSKI, Ignacy
14:10	[95] The degradation of phosphate derived ligands in hydrometallurgical solvent extraction	Mr JANSEN VAN VUUREN, Daniel
14:30	[171] A DFT study of the ODH of n-hexane over isolated H <sub>3</sub> VO <sub>4</sub> and H <sub>4</sub> V <sub>2</sub> O <sub>7</sub>	Dr DAMOYI, Nkululeko