

# Chemical Purification, Analysis and Screening (CPAS) core facility

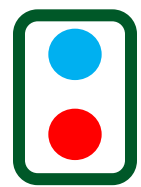
Laurent Calcul, Ph.D.  
Director

&3\$6 RIIHUV LWV H[SHUWLVH LQ FKURPDWRJUDSKLF VHSDUDWLRQ DQG SXULILFDW LGHQWLILFDWLRQ DQG TXDQWLILFDWLRQ /& 06 64 /& 06 4T4 /& 06 72) /& 06 47R) 7 >+6 630(@ DQG 0\$/', 72) 7KH VHUYLEFHV DOVR LQFOXGH &LUFXODU 'LFKURLVP &' 9 VSHFWURVFRSLF FKDUDFWHUL]DWLRQ 89 )7,5 O\RSKLOL]DWLRQ EHQFKWRS DQG JH ([WDFWRU >\$6(@ PLFURZDYH UHDFWRU V\QWKHVLV PLFURZDYH UHDFWRU K\GURJ 0HPEUDQH 3HUPHDELQW\ >3\$03\$ \*,7 %%% DQG VNLQ@ DQG GUXJ VROXELOLW\ H 7KHUPRSKRUVLV >067@ DQG KLJK WKURXJKSXW VFUHHQLQJ GHYHORSHPHQW FDSDE &3\$6 SURYLGHV WUDLQLQJV DQG LQVWUXPHQWV DUH DYDLODEOH LQ VHOI VHUYLEFH

(PD±OFDOFXO#XVI HGX :HE ± KWWSV ZZZ XVI HGX DUWV VFLHQFHV GHSDUWPH

Location site 13720 Spectrum Blvd LDRB, Suite 18 Tampa, FL 33612 <> Office (813)-0112

Location site 24202 E. Fowler Ave, NES 40 Tampa, FL 33620 <> Office (813)-0031



## Liquid Chromatography Mass Spectrometry (LC -MS)

High Resolution Mass Spectrometry (HRMS DQG DFFXUDWH 06 06)

Agilent 1200 LC/ 6540 QT 2F MS and 6230 T 2F

- HRMS for Formula determination (organic small molecules to proteins)
- Identification (using the Metlin library)
- Metabolomics capability

### Modes and Features:

- ESI (positive or negative mode)
- Agilent Jet-stream Electrospray Ionization
- Software: Mass Hunter Workstation

### High sensitivity in triple quadrupole LC/MS/MS

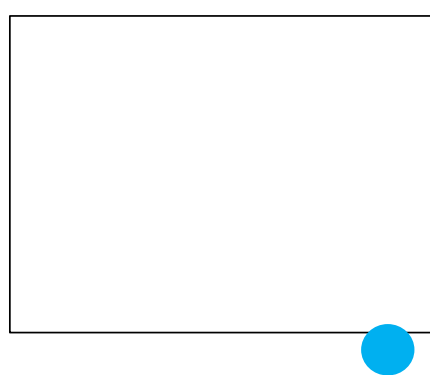
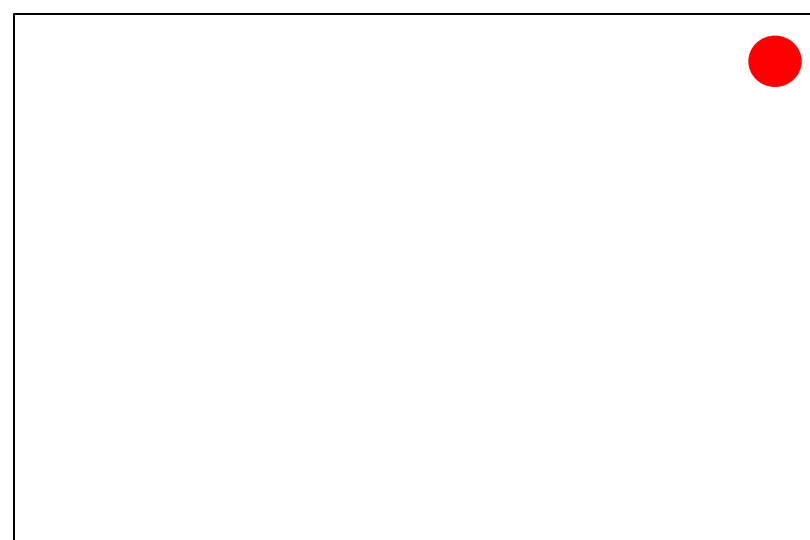
Agilent 1200 LC/ 6460 QqQ MS

- Multiple reaction monitoring (MRM) ideal for Quantification
- Sensitivity (Femtomole to Attomole range)

### Preparative Mass Spectrometry

- 1) Analytical Agilent 1200 infinity HPLC/ DAD/ SQ MS
  - Fast switching ESI (+/-)
  - Diode array detector (DAD, 190-600 nm)
  - Autosampler and fraction collector

- 2) Preparative Agilent 1200 infinity HPLC/ DAD/ SQ MS
  - Fast switching ESI (+/-)
  - Diode array detector (DAD, 190-600 nm)
  - Autosampler and fraction collector



## Gas Chromatography Mass Spectrometry (GC -MS)

High Resolution Mass Spectrometry (HRMS DQG DFFXUDWH 06 06)

Agilent 7890A GC/ 7200 QToF MS

- HRMS for Formula determination
- Identification
- Metabolomics capability
- Quantification capability

### Modes and Features:

- EI, PCI and NCI
- 10 PLsyringe, +6



Agilent 7890B GC/ 5977B SQ MS

- Selected ion monitoring (SIM)

```
*HUVWHO 0XOWL3XUSRVH 6DPSOHU 036
x 'XDO KHDGHG IRU VDPSPH SUHSDUDWLRQ
V\ULQJH +6 P/ V\ULQJH RU 630( ILEHU
x FROG LQMFWLRQ V\WHP &,6 XVLQJ /1
x 7'8 XVLQJ $/ (; IRU 7ZLVWHU 6WLU %DU
6%6( 7) 630( DQG GHVRUSWLRQ OLQHU
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Low Resolution Mass Spectrometry (LRMS)

Agilent 7890B GC

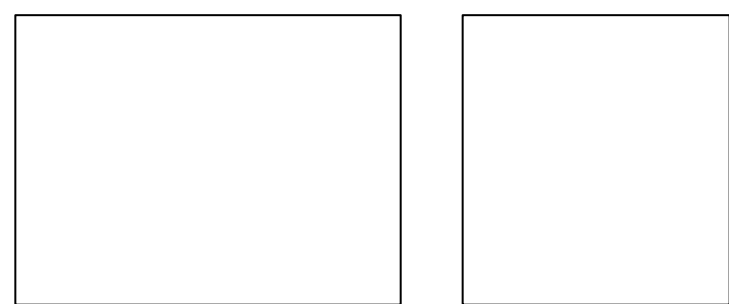
## Medium to Ultra High Performance Liquid Chromatography

- Large scale from 0.5 to 300 g
- TELEDYNE-Isco Torrent (UV 200-760 nm)

- Scale from 200 mg to 33 g:
- TELEDYNE-Isco Rf (UV 200-360 nm)

- Shimadzu semi preparative HPLC for sample fractionation and purification (UV, ELSD and RID)

- Fisher Scientific Dionex Ultimate 3000 UHPLC (DAD)



## Matrix Assisted Laser Desorption Ionization (MALDI)

### MALDI TOF and TOF/TOF technology

Bruker UltraFlex extreme MALDI

- Protein, peptide, lipids, small molecule and polymer
- MALDI Top down sequencing (TDS)
- ,PDJLQJ 0\$/', 06,

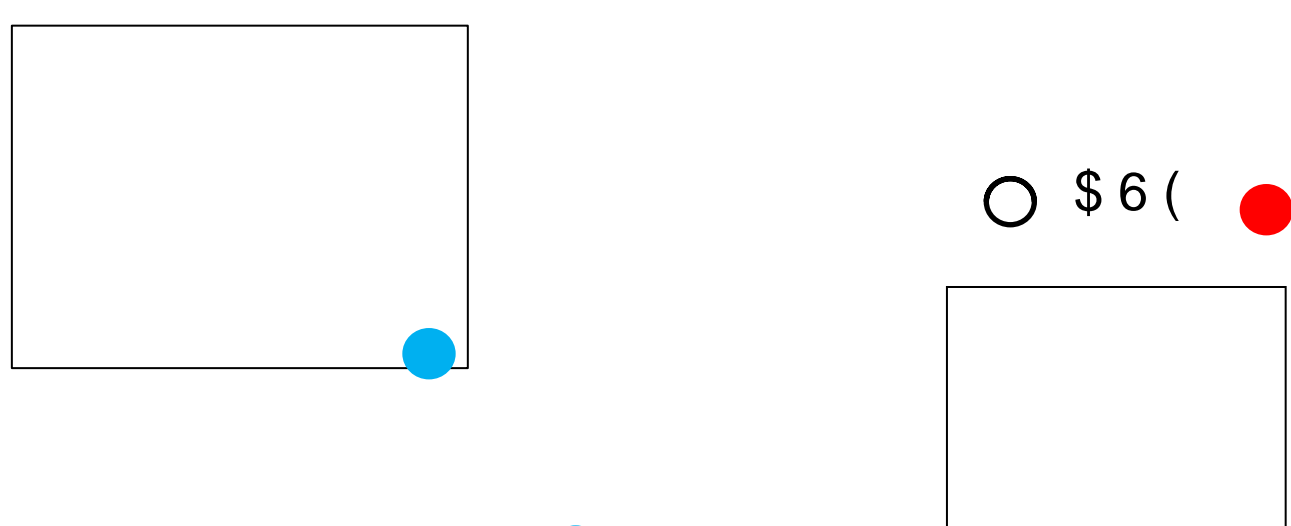
### Modes and Features:

- 06 OLQH DU UHIOHFWRU 06 06 /,)7 PRGHV
- 6PDUWEHDP ,, \*+] IRU 06 DQG \*+] IRU 06 06
- Resolution > 45,000

## ADME (PAMPA), solubility and HTS capability

- 3\$03\$ VHWV \*DNLWURLQWLFVFL@ DQG %ORRG EUDLQ EDUULHU >%%% @
- 6ROXELOLW\ HYDOXDWLRQ
- 7HFDQ )UHHGRFDXWR PDWHG OLTXLGLQ € @ •8ñ D #(u, Ef' @ 1" 6Fb v™/••:h ç "5 IA • SA p €Á( D €p Á4• DO DOHG A(Ä u u,q Ä b @ ‡GOLRQ

CPAS is a convenient platform to assist investigators in natural product chemistry (extraction, lyophilization, chromatography, spectrometry, spectroscopy), medicinal chemistry (microwave assisted reaction, ADME screening), as well as biology (storage, HTS development) for Drug Discovery:



Spectroscopy

- &' -\$6&2 >(@ & %LRWRRQVROSHQW SXULILFDWLRQ&IUHH]H&&ROG URU&RUHH]HU

- )7,5 \$JLOHQW\$&DU\ - +\$GWRCHQDDWLRQDFFXUDWH%HQFKWRSJHDSDFLW\IUHH]HGU\HUV - )XPHKRRG

- 89 \$JLOHQWIEHULF - +\GURJHQDWLRQDSSDUWRWU\HYDSRUDWRU

- \$FFHOHUDWRU VROYHQW HIWUDFWRU

General lab use:

- %HQFK

- )XPHKRRG