**The Pasarow Mass Spectrometry Laboratory** (PMSL, on the web at http://massspec.chem.ucla.edu/)

**Location:** CHS Semel Institute occupying rooms 68-162, 68-146, 68-145, 67-357 and 78-144.

**Personnel**

Kym Faull, Ph.D., Emeritus Professor on recall and Director

Julian Whitelegge, Ph.D., Adjunct Professor and Associate Director

Wanrong (Lucy) Gao, BS, Laboratory Assistant II

Alexander Jae Yoon, MS, Staff Research Associate I

Whitaker Cohn, BS, Graduate Student

Adrian Gomez, BS, MS, Graduate Student

Annie Tagvoryan, Undergraduate volunteer

Sarah Bui, Undergraduate volunteer

Arbaaz Patel, Undergraduate volunteer

Leat Kohanzadeh, Undergraduate volunteer

Vivian Le, Undergraduate volunteer

Savannah Novencido, Undergraduate volunteer

**Function**

The PMSL is an as the analytical resource for the UCLA Cannabis Research Initiative and serves as a core mass spectrometry laboratory for the entire UCLA campus and beyond. It also serves as a teaching venue to provide instruction in analytical chemistry. Teaching others, most importantly the next generation of scientists, is a crucial role the facility fulfills. The work in the laboratory can be broadly broken into two components: these are work involving small molecules (metabolites, drugs including cannabinoids, and metabolomics), and proteins including both top-down and bottom-up proteomics.

**Samples**

Serum, plasma, CSF, saliva, urine, semen, tissue homogenates, breast milk, faeces, cell cultures (cells and media), bone. Methods to analyze other samples are being developed including hair and nail clippings.

**Small molecules: quantitative assays**

Cannabinol (CBD), tetrahydrocannabinol (THC) and related compounds including (−)-trans-Δ9-THC, tetrahydrocannabivarin, Δ9-tetrahydrocannabinolic acid, (±)-11-hydroxy-Δ9-THC, (±)-11-nor-9-carboxy- Δ9-THC, cannabidiolic acid, 7-hydroxycannabidiol, and cannabidivarin (this list is being expanded).

Curcumin and related compounds, including dimethoxy-, bisdemethoxy- and tetrahydro-curcumin and their glucuronidated metabolites.

Amino acids including tyrosine (*o*-, *m*- and *p*-isomers), glutamic acid, cysteine, cystine, NAA, GABA, and many more.

Amines including kynurenine, kynurenic acid etc

Polyamines including putrescine, spermine and spermidine.

Peptides including oxidized and reduced glutathione, NAAG, gut- and neuro-peptides (PYY, CCK), cyclosporins etc

Drugs, many including risperidone, aspirin, dexamethasone, metformin. GBH and many more

Lipids, too numerous to list individually but including neutral, positively- charged (choline containing) and negatively-charged (carboxylated and sulfated) species, prostaglandins and related compounds (including 5-HETE, 12-HETE, 15-HETE, 9-HODE, 13-HODE, TXB2, PGD2, PGE2, arachidonic acid, linoleic acid, LBT4, etc) endocannabinoids (AEA [*N*-arachidonoyl ethanolamide] and 2-AG [2- arachidonoyl glycerol]), etc

Terpenes

Nucleosides, nucleotides and related compounds, including ATP, ADP, AMP, A, NAD, NADH, GppG, etc

Coenzyme Q including Q9 and Q10

Pesticides including most of those listed on the California Bureau of Cannabis Control regulations.

Naturally-occurring plant antibiotics including fengycin and related compounds

**Proteins**

Intact protein mass measurements & top-down mass spectrometry

Peptide mapping and bottom-up mass spectrometrys

Protein post-translational modifications

Non-covalently bound protein ligands including endogenous and exogenous (drugs) ligands

**Facilities**

*Space:* The UCLA Pasarow Mass Spectrometry Laboratory occupies three laboratories (around 2,000 sq.ft total) and two shared-facility rooms (housing -20ºC and -80ºC freezers and vacuum centrifuge equipment ) on the 6th floor of the Semel Institute the UCLA Center for Health Sciences (CHS). The space is equipped with all the necessary facilities required for sensitive analytical instrumentation and wet chemistry, including fume hoods, house air, vacuum and gas, and additional lines to supply other essential gases (nitrogen, zero air, argon and helium). A spacious walk-in cold room is conveniently located nearby and a walk-in freezer (-20ºC) is conveniently located on the fourth floor of the building

*Computing:* Modern computer facilities have been installed with Terabyte connections to the entire campus and elsewhere.  The PMSL is equipped with several laboratory computers including PC, Macintosh, and Linux systems. Numerous workstations for lab personnel are also available to accommodate undergraduate, postgraduate, postdoctoral fellows, faculty and staff. Computing and informatics capabilities include a central data storage of more than 10 Terabytes (TB) to store all data. The storage server is a dual processor, quad core linux server with 8 GB of RAM and is accessible throughout UCLA via secure and encrypted protocols. The server is hosted in the UCLA Academic Technologies Services (ATS) data center. Overnight syncing backups are also maintained in the laboratory and remote backups are also maintained on tape. A computational server with dual hex cores and 16 GB of RAM hosting virtual machines is available for a variety of both top-down and peptide data analysis.

Available metabolomics software packages include the Waters *MarkerLynx* subroutine (this is a sub-routine associated with the *MassLynx* software), *XCMS* that is an on-line package developed at The Scripps Research Center, *Progenesis CoMet - Metabolomics* Software package from NonLinear Dynamics, and an in-house developed software package (as yet un-named).

Protein and peptide database searches are most frequently made using the Mascot (Matrix Science) search engine, although Sequest (Thermo-Finnigan), OMSSA (NCBI), InsPecT (Center for Computational Mass Spectrometry) and X!-Tandem (The Global Proteome Machine) are also used. OMSSA is available through the UCLA grid (http://grid.ucla.edu) and jobs can be run on a local cluster in addition to the UCLA grid computer nodes. Scaffold (Proteome Software) is available for label-free quantitation via spectral counting. Progenesis LC-MS (Nonlinear Dynamics) is also used for label-free quantitation via signal intensity.

For “Top-Down” data analysis, an internal Prosight PC running over dual Xeon processors is used in addition to Prosight PTM (https://prosightptm.scs.uiuc.edu/). Peak lists are generated using XtractAll (Thermo).  In addition to the above computing resources, web and secure FTP servers are used to host the PMSL electronic sample submission system and the PMSL homepage (http://massspec.chem.ucla.edu/). All server based computing resources are hosted on gigabit connections in data centers with redundant backup power

*Equipment including ten mass spectrometers*

1. A Thermo Q Exactive GC/MS system (provides sub ppm mass accuracy) with a Trace 1310 GC and a TriPlus RSH (Leap) autosampler with interchangeable standard split/splitless Grob-type, headspace and SPME injector modules.

2. Two Agilent 6460 triple quadrupole LC/MS systems, one equipped with an Agilent 1290 Affinity UHPLC and interchangeable Jet Stream and APCI sources, and the other attached to an Agilent 1200 HPLC and equipped with the Agilent electrospray ion source.

3. A Thermo Q Exactive+ LC/MS system interfaced interchangeably with either an Eksigent NanoLC-2D or a Thermo Ultimate 3000 LC for nanobore- or analytical-scale in-line chromatography, respectively.

4. A Thermo LTQ Orbitrap XL LC/MS system with a Finnigan Surveyor MS HPLC pump (binary) and a Thermo/Finnigan Micro AS autosampler.

5. A Finnigan LTQ interfaced interchangeably with either an Applied Biosystems 140B solvent delivery system for manual injections, or an Agilent 1200 series binary HPLC with degasser, diode array detector (DAD) and autosampler. Used principally for top-down proteomics experiments.

6. An ABI DE STR MALDI-TOF mass spectrometer.

7. A Thermo LTQ XL orbitrap LC/MS system interfaced with an Agilent 1100 series binary HPLC with autosampler (to be installed shortly).

*Stand-alone HPLC equipment includes:*

1. Two HP 1090 Series II Chemstations with DAD modules.

2. A Shimadzu Prominence HPLC system with communications, quaternary pump, degasser, manual injector, autosampler, UV/Viz, DAD and fluorescence detector modules, and an inbuilt fraction collector.

3. An Agilent 1100 series binary HPLC system with pumps, degasser, oven heater and DAD.

General laboratory equipment includes all that is required for the proposed experiments including centrifuges (Beckman Coulter Allegra**™** 25R, microcentrifuges (Eppendorf 5418, Sorvall Biofuge, etc)), refrigerator/freezer units (2), freezers (two -20°C, two -80**°**C), a vacuum concentrator (Savant SpeedVac**®**, 4 centrifuge units connected to the same liquid nitrogen cold trap, capable of accommodating a variety of tube sizes up to 50 mL Falcoln tubes), and a nitrogen drying apparatus.

The laboratory also has additional electrochemical (BAS model LC-4B) and fluorescence (Shimadzu and McPherson SF-749) HPLC detectors. A 1D-gel system is available, and a 2D-gel and related equipment including an Amersham Pharmacia DALT 2D gel system is now located in the Molecular Instrumentation Center, about a 10-minute walk from the PMSL.