1999-2000
MASS SPECTROMETRY AND PROTEIN STRUCTURE LABORATORY
SUMMARY OF ACTIVITIES

I. PUBLISHED ABSTRACTS

Ann Abraham, Walter H. Wilborn, and F. Aladar Bencsath. GC/MS Determination of Acetone in Soft Drink Using Different Headspace Techniques. Proc., 47th ASMS Conf., Mass Spectrometry and Allied Topics, #162 (1999).

II. PRESENTATIONS

F. Aladar Bencsath. Sensing Petroleum in Fish With the Electronic Nose. The Gulf of Mexico Symposium, Mobile, AL (2000).

Ann Abraham. Preparation of Irreversibly Sickled b-actin From Normal Red Blood Cell b-actin Verified by Liquid Chromatography and Off-line Mass Spectrometry. 48h ASMS Conf., Mass Spectrometry and Allied Topics, Long Beach, CA (2000).

F. Aladar Bencsath. Hydrocarbon Analysis in Tainted Salmon by the Use of Electronic Nose and Dynamic Headspace Gas Chromatography/Mass Spectrometry. 48h ASMS Conf., Mass Spectrometry and Allied Topics, Long Beach, CA (2000).

III. BRIEF SUMMARY OF ACTIVITIES

1. Personnel. No change in personnel occurred during this year: Dr. Ann Abraham, Research Associate, half-time employee, and Dr. F. Aladar Bencsath, Director, employed by the Food and Drug Administration, met the service and collaborative research obligations.

2. Service. In the past year, 516 samples were submitted for analyses by 20 investigators from 14 laboratories: 15 investigators from 9 laboratories in the College of Medicine, 4 in non-medical departments at the University of South Alabama, and 1 outside the university. The analyses required 978 instrument hours, of which about 250 hours were spent for instrumental & method development. Instrument maintenance also required about 100 hours.

The largest portion of the samples required electron or chemical ionization (314; 61%), and another large portion required fast atom bombardment ionization (153; 30%). A few samples required accurate mass/elemental composition determination (8; 2%), and MS/MS analyses (2; 0.4 %).

Samples from two research projects required gas chromatography-mass spectrometry (GC/MS) analyses with electron ionization (261; 50 %), and a third one required GC/MS with electron capture negative chemical ionization (51; 10 %). For these samples, specific clean-up and GC processes were developed, which were carried out in collaborative efforts. To determine the volatile trace components in 16 seafood samples (3%), dynamic headspace enrichment techniques were utilized in combination with GC/MS analyses.

3. Collaboration. We continued the collaborative research with Dr. Steven Goodman, Director of the Comprehensive Sickle Cell Center, on the oxidative transformation of ß-Actin in order to produce the Actin specimen equivalent to the irreversibly sickled cell ß-Actin, which plays a pivotal role in irreversible sickling. This modified protein is needed for biochemical studies that aim to inhibit and reverse the sickling process.

In the course of another collaboration, with P.I. Dr. Michael Chicella, Pediatrics, we have developed a GC/MS method for propylene glycol analysis in blood and urine of children administered with the tranquilizer lorazepam.

In the third collaboration, with Dr. Michael Zayek and Ms. Martha Stober, Neonatology/Pediatrics, another GC/MS method was implemented for lactulose/mannitol analysis in urine and milk in order to evaluate the intestinal permeabilities of very low birth weight infants. The preliminary GC/MS data of the urine samples were confirmed by a more traditional liquid chromatography/refractive index detection method.

Presently, in collaboration with Dr. Dirk Dhossche, Psychiatry, we are developing an electron capture chemical ionization GC/MS method for GABA determination in blood plasma. The novel electronegative GABA derivative demonstrates excellent MS and GC characteristics needed for the analyses at the nanogram level. We should only improve the plasma cleanup procedure to accurately accomplish the analytical process on samples from autistic and normal children.

An earlier collaboration on the FDA project "Petrochemical hazards in seafood" was continued using dynamic headspace GCMS analyses, sensory assessment and "electronic nose" instrumentation. Selective absorption of the mono- and bi-cyclic aromatic hydrocarbon compounds by fish and oyster from petroleum contaminated water were demonstrated. The dominant components may be useful markers of petrochemical taint in seafood after oil spill.

Three of these collaborations have produced data in sufficient amount and quality for future research papers.

4. Training. Ms. Martha Stober obtained training for the use of HPLC and GCMS to analyze mono- and disaccharides in milk and urine. Dr. Lorna Bland (Psychaitry resident) obtained training in chemical derivatization of GABA in plasma, and in electron capture ionization GCMS.

5. Future direction. The increased number of collaborative projects is a good indication of the increased awareness of our Faculty about the analytical help mass spectrometry can provide. Three of these collaborations used GC/MS techniques. An earlier survey, and the frequent inquiries by present and prospective faculty members also show the increasing importance of the biopolymer analysis, which requires liquid chromatography combined with either electrospray or laser desorption mass spectrometer (LC/MS).