## DRUG CHEMISTRY TRAINING MANUAL

## **APPENDIX B: Study Guide**

The study guide is not all encompassing. It is general knowledge based and questions and discussion topics may be modified by Technical Lead as needed.

### LABORATORY SAFETY

- 1 Where can safety guideline be found for the lab?
- 2 Are all safety guideline in one document?
- 3. What inherent risks can be found in the lab?
- What are MSDS and where are the stored.
- 4 What products are used for solvent, acid and base spill?
- 5 Can the same product be used for all three?
- 6 Who should be notified of a safety issue?
- 7 What types of safety training is provided for your protection?
- 8 What safety equipment is provided for your protection?
- 9 Does any safety equipment require training?
- What safety equipment should be worn for the following incidents;
  - Acid spill in the fume hood
  - Solvent spill on the floor
  - Base spill on the counter top
  - Acid spill in the sink
  - Large volume of powder spill on workbench
  - Biological spill on counter
- 11 What type of disinfectant should be used for a biological spill?
- What are some of the common errors that occur while wearing gloves that exposure you and others to contaminants?
- 13 Compressed gases:
  - What type of cylinder and gases are used by the lab? What is the purity level of the gases used?
  - Where are cylinders stored and what is the proper method for storage:
  - How do you properly transport gas cylinders?
  - What is the proper method to check gas system for leaks?

### LEGISLATION

1 When is the Texas Legislation

- In session:
- Out of session:
- Special Session:
- Who can call for a special session?
- 3 What department or governing body determines
  - Which schedule to assign to a drug.
  - Which penalty group to assign to a drug
- 4. What department or governing body determines if a substance is a controlled substance?
- 5 Are federally controlled substances automatically controlled by state law?
- What is the name of the Act that determines if a drug is illegal?
- Are there any drugs that are both legal and illegal?
- 8 How are new laws created?
- 9 What is a pending law called?
- 10 How can you check on a pending law?
- 11 How are new laws published?
- 12 Bookmark website containing the Texas Controlled Substance Act.
- The Texas Controlled Substance Act is found in the Health and Safety Code. Under What Title, what sub-title and what chapter?
- What other chapters would pertain to suspected drugs?
- 14 Bookmark website containing list of federally controlled substances.

# **Quality Assurance/Ethics**

- 1 What does quality assurance (QA) mean?
- What is the Bureau quality assurance plan and where can it be found?
- 3 What quality assurance measures are taken equipment used for drug analysis?
- 4 What QA measures are taken for work conducted before reports are issued?
- 4 What corrective actions can be taken to address a QA issue?
- 5 Who is responsible for QA?
- 6 Is there a difference between ethic and forensic ethics?
- Read the National Academy of Science (NAS) Report. What ethical dilemmas lead to the NAS Report?
- 8 How does the Texas Forensic Science Commission (TFSC) relate to forensic QA and forensic ethics?

- 9 Read "Certification of Forensic Examiners in Texas" a white paper by TFSC. What is the difference between certification and accreditation?
- Become familiar with ASCLD/Lab requirement, ISO 17025 requirements, Bureau and section requirements for QA.
- What are the limitations set by forensic ethics? What should a forensic professional refrain from doing?

## **COURTROOM TESTIMONY**

- 1 Discuss the role of the following during a trial:
  - Expert witness
  - Judge
  - Prosecutor
  - Defendant
  - Defense counsel
  - Jury
  - Judicial Jurisdiction
- 2 Define the following:
  - Voir dire
  - Direct examination
  - Cross examination
  - Redirect
  - Chain of custody
  - Felony
  - Misdemeanor
  - Jury Panel
  - The Rule has been involked
- 3 Complete a current curriculum vitae in the format provided by the Bureau which should include educational background and work experience.
- 4 Produce a flow chart of a typical courtroom proceeding for your portion of the testimony for the trial of an individual accused of a single item of possession of a controlled substance,. Be sure to include the order how evidence reaches the court and how it is introduced and by whom and what arguments by trial counsel, are asked by whom.
- How would you describe the characteristics of an effective expert witness? Likewise, what are some factors which make a poor expert witness?
- 6 Describe the ASCLD/LAB accreditation process and the benefits of being an accredited laboratory
- 7 Practice questions for jury trial
  - What is your name?
  - What is your occupation? For whom do you work?

- How long have you been so employed?
- What are your duties in this occupation?
- What education and training do you possess that qualifies you to perform your duties?
- What specific courses have you taken that are directly related to drug analysis?
- How are these courses related? For example, what did you learn in your general chemistry course that aids you in the analysis of drugs?
- Do you consider yourself an expert in the analysis of drugs?
- What is the definition of an expert witness?
- Who conducted your training?
- What are his/her/their qualifications?
- What literature do you read relating to your job?
- How many analysis have you done on suspected drugs (or controlled substances)?
- Do you belong to a recognized society attesting to your qualifications as a drug chemist?
- Have you written any articles or published materials dealing with your work?

## **EVIDENCE HANDLING**

- 1 Explain the parallel chain of custody methods used by the Bureau.
  - Receipt and transfer of evidence using LIMS
  - Creation of new items into RMS
  - Linking items from RMS to LIMS
  - Creation of new sub-items in LIMS
- 2 Define a proper seal.
- What is the proper way to mark evidence?
- Who has access to the main evidence storage room? Who has access to your temporary storage area? The drug vault cabinet room?
- 5 Describe the procedures for access to your locker in your absence.
- 7 Explain the central evidence lock box procedure? Where is the key housed? Who has access to this key?
- 8 Explain how to handle evidence which also needs a latent print analysis.
- 9 Explain how to handle evidence which also needs a DNA analysis.

### **BALANCES**

- 1 Define the following:
  - Accuracy
  - Precision
  - Balance
  - Analytical balance
  - Certified weight
  - Tare
  - Trace amount / Residue

- Truncate
- 2 Explain the quality assurance program for balances in the Forensic Chemistry section. How is it documented?
- 3 Is balance calibration done with an internal or external weight?
- 4 What types of weights are used to balance QA? Are they traceable?
- 5 What is the accuracy of the balances in your laboratory?
- What is the mathematical conversion between grams and ounces? Pounds?
- 7 What is the difference between the troy and avoirdupois weight systems?

## SAMPLING AND UNCERTAINTY

- 1 Define the following:
  - Sampling
  - Statistic
  - Population
  - Sample
  - Homogeneous
  - Heterogeneous
  - Aliquot
  - Random
  - Representative
  - Arbitrary
  - Selective
  - Coning and Quartering
  - Grab Sample
  - Sampling without replacement
  - Sampling with replacement
  - Weight fraction
- 2 Define normal distribution, binomial distribution, and hyper geometric distribution.
- What is the purpose of sampling?
- 4 What physical properties of particles must be considered when sampling powders?
- 5 What is a "composite" sample? When is it acceptable to do a composite?
- What criteria must be used to determine the size of the sample?
- 7 Outline sampling protocols used in the laboratory.

## DRUGS OF ABUSE

### **CANNABIS**

1 What is the definition of marihuana as per Texas law? As per federal law?

- 2 Describe the appearance of a mature marihuana plant.
- 3 What is the derivation of the word marihuana?
- 4 What is sinsemilla and how is it grown?
- 5 What is hemp?
- What is the scientific name for marihuana including family, genus and species?
- 7 What parts of the plant contains THC?
- Befine "agronomic variety" and differentiate between Cannabis sativa, Cannabis ruderalis, Cannabis indica and Cannabis Americana.
- 9 Define dioecious and relate to Cannabis. Include the different morphological characteristics between the two.
- 10 What is the function of the resin found on the plant?
- 11 Describe the differences between hashish and hash oil including preparation and analysis?
- 12 Is there any difference in penalty between marihuana, hash and hash oil?
- What is the pharmacological classification of marihuana?
- 14 Define the following:
  - Cannabinoids
  - Alkaloids
  - Parahexyl
  - Synhexyl
  - Dronabinal
- 15 What factors influences the relative amounts of cannabinoids present in marijuana?
- What are the two numbering systems for cannabinoids in use today? Draw THC and show how these numbering systems differ.
- 17 What types of isomers are delta 9-THC and delta8-THC? Which is more stable?
- 18 Is d-THC or I-THC the naturally occurring isomer?
- 19 Are the cannabinoids acidic or basic? Polar or non-polar?
- 20 Chemically, can any of the other cannabinoids break down or be converted to THC? Does THC break down?
- 21 What information is gained from the macroscopic examination?
- What power of magnification is needed to view cystolith hairs and glandular hairs?
- 23 Describe cystolith hairs including characteristics and locations found on marihuana.
- 24 Describe glandular hairs including characteristics and locations found on marijuana.
- 25 How can you distinguish between marihuana cystoliths and cystoliths on other plants?
- Discuss any other plants which have cystoliths including how to differentiate them from those on marijuana.
- What is a screening test?
- 28 What substances give false positives for Duquenois-Levine test?
  - Coffee (ground, freeze dried, liquid)
  - Patchouli oil
  - Peppermint oil

- Secret cough drops
- Sandalwood Oil
- Other substances and plants provided
- 29 What causes the purple color obtained with the Duquenois reagent and marihuana?

## **GENERAL DRUGS OF ABUSE**

- 1 Define the following:
  - Controlled Substance
  - Drug
  - Dangerous Drug
  - Over the Counter Drug
  - Distribution
  - Manufacture
  - Marihuana
  - Amphetamines
  - Cocaine
  - Hashish and hashish oil
  - Anabolic steroid
  - Narcotic
  - Opiate
  - Hallucinogen
  - Depressant
  - Stimulant
  - Alkaloid
  - Cis- and trans- isomers
  - Optical isomers
- 2 Match the following drugs with their state classification, scheduling and penalty group: Classification: AS – Anabolic steroid; D – Depressants; H – Hallucinogen; N – Narcotic/Opiate; S – Stimulant

Drug	Classification	Schedule	Penalty
		Group	Group
3,4-MDMA			
PCP			
Heroin			
Hydromorphone			
Psilocyn			
Methadone			
Pentobarbital			
Salicylamide			
Codeine			

Nandrolone Decanoate	
Methamphetamine	
Caffeine	
Diazepam	
Cocaine HCI	
Dextropropoxyphene	
Meperidine	
Phentermine	
Chlordiazepoxide	
DMT	
Oxycodone	
Methylphenidate	
GBL	
Trenbolone implants	
LAMPA	
Ethanol	
Benzocaine	

- 3 List the physiological effects of the following:
  - Designer drugs
  - Depressant
  - LSD
  - Anabolic steroids
  - Phenethylamines
  - Morphine
  - Analgesics
- 4 List the pharmacological actions of the following drug classes:
  - Depressants
  - Hallucinogens
  - Narcotics
  - Stimulants
- 5 Depressants
  - What is the difference between a sedative and a hypnotic?
  - What is the largest drug group within the depressants?
  - How are barbiturates classified?
  - Draw the general structure of a barbiturate.
  - How are most depressants illegally obtained?
  - Why are the benzodiazepines includes with the depressants? Give their general structure.
  - What is chloral hydrate and how is it used and how is it abuse?
  - Explain the relationship between GHB, GBL and 1,4-butanediol.

 Describe the equilibrium formed between GHB and GBL in aqueous solutions of various pH values. How does this affect the analysis?

## 6 Hallucinogens

- What medicinal use do hallucinogens have?
- From what is LSD derived?
- What is the chemical name for LSD?
- What is peyote? Is it controlled? What is the active ingredient in peyote?
- What is the scientific name for "magic" mushrooms?
- What is the chemical name for MDA? For MDMA? For MDEA?
- What is the chemical name for PCP? How are the letters of PCP derived from the chemical name?
- Describe a synthetic route for the clandestine manufacture of PCP?
- What is the legal use of PCP?
- What are the chemical names of DMT and STP?
- What is the structural similarity between STP and MDA?

### 7 Narcotics

- Define a narcotic according to The Texas Controlled Substance Act.
- From what plant is opium obtained? How? Where is the major crops grown?
- What is the major difference between Heroin found in northern states versus southern states?
- What is the definition of an opiate?
- What are the classification of opium alkaloids and how they differ?
- What percentage (by weight) of opium are alkaloids?
- How many alkaloids are in opium and which is the principal constituent?
- Name the principal narcotic drugs.
- What is the chemical name for Heroin? Street name?
- Define and give examples of each
  - Natural opiate
  - Synthetic narcotic
  - Semi-synthetic narcotic
- How are narcotics used or administered?

### 8 Stimulants

- What are the two most common stimulants abused?
- Draw the structure of phenethylamine.
- What are the major uses of amphetamines?
- How is the word amphetamine derived?
- Name some amphetamine-related stimulants.
- Describe three different synthesis methods for methamphetamine.
- What is an anorectic drug?
- What are some street names for some commonly encountered stimulant?

- When is cocaine classified as a stimulant? As a narcotic?
- From what plant is cocaine obtained from? Where is the major crop grown?
- How is cocaine base produced from cocaine hydrochloride? How does "crack" differ from "freebase"?
- How are various stimulants used or administered?

### 9 Miscellaneous

- What is physical dependence and how does it vary from psychological dependence?
- What is meant by tolerance?
- What are some common household items with a high potential for abuse?
- Define the following drug actions:
  - Analgesic
  - Antipyretic
  - Antitussive
  - Tranquilizer
  - Anti-cholinergic
  - Vasoconstrictor
  - Anti-hermitic
  - Diuretic
  - Bronchodilator
  - Antibiotic
  - Vitamin
  - Anesthetic
- What is the difference between an antidepressant and a stimulant?
- Name four common tricyclic antidepressants.
- What is the difference between and anabolic steroid and a corticosteroid?
- Describe the following terms as if you were addressing a lay audience or jury panel:
  - Stimulant
  - Anesthetic
  - Antibiotic
  - Hallucinogen
  - Designer Drug
- 11 What is a drug free zone? Name locations at fall into this category?
- What are the cut off weight for controlled substances for the different penalty groups and marihuana?
- 13 Is there a difference for possession and delivery?
- 14 Does the possession in a drug free zone influence the penalty range?

### PHARMACUETICAL IDENTIFCATION OF DRUGS OF ABUSE

Name the various pharmaceutical references used by the section.

- Where is the approved list of pharmaceutical references listed?
- Name a manufacturer, the active ingredients, and active non-narcotic ingredients of the following preparations:

Brand	Manufacturer	Active Ingredient	Non Active Ingredient	Imprint
Oxycotin			Ingredient	
Adderall				
Preludlin				
Demerol				
Ritalin				
Keflex				
Zoloft				
Percodan				
Darvon				
Darvocette				
Lortab				
Vicodin				
Vicoprin				
Xanax				
Clonopin				
Viagra				
Soma				
Valium				
Fiorinal				
Wellbutrin				

- What information should be recorded in the case notes to ensure proper documentation of visual examination?
- When and why should screening tests be performed on tablets or capsules along with the visual examination?
- 5 How does the analysis of an injectable dosage form differ if tampering is suspected?

## **COLOR TESTS**

- 1 Where can the recipes for each of the following color test reagents be found?
- 2. List the types of compounds that react with each test, and state what reaction would be observed:
  - Marquis
  - Meckes
  - Froehdes
  - Cobalt thiocyanate
  - Ehrlich's TBPEE

- Dille-Knoppanyi
- Ferric chloride
- Stannous chloride
- Sodium nitroprusside
- 3 Do any of the above color tests go by another name?
- For the following color test reagents, what would be an appropriate compound for QA purposes in laboratory?
  - Marquis
  - Cobalt thiocyanate
  - Sodium Nitroprusside
  - Duquenois
- 5 Describe as to a jury how a color test is performed, including the purpose and value of the test.
- An officer calls stating that field test kit used on a submitted sample indicted the presence of heroin. Your analysis reveals no controlled substances. How might you explain this?
- 7 Briefly describe the mechanisms of the following tests:
  - Marquis
  - Cobalt thiocyanate
- 8 Describe the difference between the terms "sensitivity" and "selectivity" as they relate to color tests.
- 9 What is the definition of presumptive and confirmatory?
- 10 Are color test results presumptive or confirmatory?
- 11 Define "false positive". Give three examples of false positive color tests.
- 12 Define "false negative". What drug using which color test can give a false negative?
- What tests can be used to detect some cutting agents? What are they and what cutting agent is detected?
- 14 Describe the Scott Test?
- 15 Describe the use of blanks pertaining to spot tests.
- 16 What effect do mixtures have on spot test results?
- 17 What effect does time have on color test reagents?
- 18 Define the following terms:
  - Precipitate
  - Complex
  - Ligand
- 19 Where can the QA procedure for color test reagents be found?

## **STEREOMICROSCOPE**

- 1 Describe the various parts of the stereomicroscope and the function of each.
- 2 How does the stereomicroscope differ from other microscopes?
- 3 How is magnification determined? What magnification ranges are used in the laboratory?

## **GAS CHROMATOGRAPH**

- What is chromatography?
- 2 What types of information is obtained from GC?
- 3 Draw a schematic diagram for GC and describe the purpose of each component.
- 4 Define the following terms:
  - Resolution (R)
  - Carrier gas
  - Mobile phase
  - Partition
  - Volatility
  - Distribution coefficient
  - Retention time
  - Retention index
  - Linear velocity
  - Flow rate
  - Injection port
  - Flame ionization detector
  - Internal Standard
  - Phase ratio
  - Selectivity
- 5 What general criteria should all stationary phases possess?
- What general criteria should all mobile phases possess?
- 7 Besides the stationary phase, what factors influence column selection for a given GC application?
- 8 What determines the appropriate column diameter for a given GC system? The appropriate length?
- 9 Describe how the following concepts affect GC separation between components:
  - Solubility
  - Boiling point
  - Drug mixtures
  - Drug in its salt form
  - Drug in its base form
- 10 What factors influences the "inertness" of a column?
- 11 What is the purpose of the polyimide/polyamide coating on a fused silica column?
- What is difference between a bonded and cross-linked phase and what are their advantages?
- 13 What is column bleed?
- When and why are columns conditioned? Describe the process.
- Define partition coefficient (K)? What is it a function of?
- How does it relate to equilibrium?
- 17 What is meant if K = 1?
- What is the partition ration/capacity ratio (k)? How does it relate to retention time?

- 19 Define the following
  - Theoretical plate (n)
  - Effective theoretical plate (N)
  - Theoretical plate height/height equivalent to a theoretical plate (H or HETP)
  - Height equivalent to an effective theoretical plate (H or HEETP)
  - Average linear gas velocity (u)
- Why is resolution not the best measure of column efficiency and column performance?
- Discuss the effects of columns i.d. and stationary phase film thickness with respect to sample capacity, column efficiency, relative retention times and resolution.
- 22 Diagram and explain the Van Deemter plot. Why does the drug lab use helium as a carrier gas?
- What two factors influence the relative retention time of two components?
- What is the Kovats retention index (I)? What does it mean if I = 650.
- What effects do the following have on retention time?
  - Concentration
  - Other compounds in the sample
  - Free base/acid form versus salt form
- 26 Discuss the sample introduction of gases and vapors, volatile liquids and solids into a GC.
- What is meant by flash vaporization?
- 28 Describe the manual injection technique?
- What factors govern the amount of sample to be injected?
- 30 How much sample/component can the average capillary column hold? What factors influence this?
- 31 What temperature should the injection port be under normal circumstances and why?
- What are the differences and purposes of "split" injection, "splitless" injection, "con-column" injection, and "direct-on-column" injection?
- What types of septa are recommended for GC work and why?
- What is the injection port liner? What is it made of? Why is it used?
- What is a "split ratio" and how is it calculated?
- What factors govern the use of a particular split ratio (100:1 vs. 50:1)?
- What is meant by linear split, why is it desirable and how is it achieved?
- Why is it necessary to regulate the carrier gas flow and how is this done?
- 39 What factors influence the optimum flow rate for a given carrier gas?
- If the carrier gas is too fast or too slow how will it affect the peak shapes of your sample components? How will it affect the detector?
- Discuss the Flame Ionization (FID) detector Electro capture) with respect to the following:
  - How does each work?
  - Carrier gas requirements
  - Sensitivity
  - Temperature requirements
  - Stability
  - Insensitivities

- Advantages/disadvantages with respect to organic drug analysis
- What is "make-up" gas? How and why is it used?
- 43 What determines which gas will be used as make-up gas?
- What is an attenuator and how and why is it used? Is it linear?
- What types of GC's (model, manufacturer, etc.) does the drug laboratory use?
- What type of injection ports, carrier gases, flows, columns and detectors does each GC incorporate?
- 47 What type of integrator(s) does the drug laboratory use? Are they mechanical or electronic?
- 48 Outline a logical troubleshooting schematic for isolating the source of a GC system problem.
- What three things can cause insufficient gas flow through a GC system?
- Describe how to change the septum on the GC's.
- 51 What are some of the problems encountered when the septum is too tight or too loose?
- What are some of the common causes and remedies for the following GC system problems?
  - No peaks
  - Solvent peak only
  - Baseline drift or unstable
  - Ghost peaks
  - Tailing peaks
  - Leading peaks
  - Split peaks
  - Baseline rise before or after a peak
  - Retention time shift
- Describe the preventative maintenance schedule and QA/QC procedures performed on the GC's.
- Discuss the operation of the autosampler.
- What is "needle discrimination" and how is it corrected?
- What is gas saver and how is it used?
- 57 What is EPC? Explain the difference between constant flow and constant pressure?
- Draw a diagram of the injection port and illustrate the carrier gas flow throughout both split and splitless injections.
- 59 Explain how derivatization is performed, including why it is used sometimes for analysis.
- Describe the internal standard method of quantitation. How accurate is the method generally?
- What is the mathematical formula for calculating purity? Define each variable.
- If two drug compounds were to co-elute on the GC, what could be done to resolve the peaks?
- Explain as to a jury how a GC operates?

## MASS SPECTROMETRY

- 1 What is mass spectrometry?
- 2 Describe the theory behind its use as an identification technique.
- 3 What types of information are obtained from GC/MS?

- 4 Draw a schematic diagram of GC/MS. What is the purpose of each component?
- 5 Define the following terms:
  - Relative abundance
  - Base peak
  - Molecular ion
  - Quasimolecular ion
  - Parent/precursor ion
  - Daughter/product ion
  - Mass/charge ratio
  - Mass spectrum
  - Resolution
  - Unit mass resolution
  - Normalization
  - DFTPP normalization
  - AMU
  - Calibration compound
  - Torr
  - Atmosphere
  - Total ion current
- 6 What is "metastable peak"? When and where does it occur?
- What is the sensitivity of a GC/MS? How do the various models of GC/MS systems in our lab compare with respect to sensitivity?
- 8 What is the difference between spectrometry and spectroscopy?
- 9 How can non-volatile compounds be introduced into a mass spectrometer?
- 10 What is the most common mode of ionizations?
- 11 Diagram the E.I. source for the Agilent 5973.
  - Are the ions formed positive or negative?
  - Do they have an even or odd number of electrons?
  - What governs the relative abundance of the ions formed?
- What governs the number and energy of the electrons emitted by the filaments?
- 13 From what are the filaments made?
- What vacuum conditions are necessary in the ionization source?
- 15 Describe how the following pumps work:
  - rough pump,
  - diffusion pump and
  - turbomolecular pump
- 16 Is it necessary that the vacuum remain constant?
- 17 What temperature conditions must be maintained in the ion source?
- Describe how the ions are accelerated once they are formed.
- 19 Describe how a quadrupole mass analyzer works.
- 20 What factors influence the practical limits of the quadrupole as a mass filter?

- 21 What determines whether an ion will have a stable trajectory through the quadrupoles?
- 22 Describe the theory of ion trap.
- 23 Define mass resolution and what is the resolution a function of?
- 24 Describe how an electron multiplier works
  - Why is it referred to as a continuous dynode?
  - What is the inner surface of the electron multiplier coated with?
- 25 Why is the electron multiplier the detector of choice and what are the limiting factors as to how well it can detect incoming ions?
- 26 Explain how the 10-peak and PBM library search routines work.
  - How many peaks are stored in a library spectrum in each?
  - How does the software decide which peaks to use?
  - What makes a peak significant to each of these searches?
  - What are the limitations of the computer library?
- 27 What is the difference between "normalized" data and DFTPP ion abundance calibrated data?
  - How is MS data usually normalized?
  - Why are perfluorinated compounds uses as calibration compounds?
  - What does DFTPP stand for?
  - What does PFTBA?
  - Why is PFTBA preferred over DFTPP as an internal calibration standard?
- 28 What reference spectra collections are available for your use?
  - Do they consist of "normalized" data?
  - Do they consist of DFTPP ion abundance calibrated data?
  - Do they contain verified data?
  - If data is not verified, are they still viable references for spectral comparisons?
- 29 List what the base peaks and molecular ions are for each of the following:
  - Cocaine
  - Heroin
  - LSD
  - Methamphetamine
  - Phencyclidine
- 30 Can ephedrine and pseudoephedrine be distinguished by MS?
- 31 Can optical isomers and diastereomers be differentiated via MS?
- Obtain a mass spectrum for cocaine and account for the major peaks in the spectrum.
- List the isotopic abundances for each of the following elements: H, C, N, O, F, Si, P, S, Cl, Br, and I.
- What is the nitrogen rule?
- If a molecular formula has been determined, how can the number of rings and double bonds be determined?
- What is the "index of hydrogen deficiency"?
- 37 What influences what bond sites will be ruptured to create molecular fragments?
- 38 Describe how fragmentation patterns are influenced by:

- Branched carbon atoms
- Double bonds
- Rings
- Hetero-atoms
- Carbonyl groups
- 39 What are or "A+2" elements?
- 40 What percentage of intensity of a molecular ion is contributed to the M+1 peak by carbon atoms?
- What is the formula for calculating the number of carbons atoms in a molecule and how can the M+1 peak be used to determine the molecular weight?
- 42 Describe the isotope pattern for Cl and Br.
- What ions can be associated with the following m/e ratios?
  - 43
  - 58
  - 77
  - 91
- Explain the terms "sequence file", "macro" and "data file".
- 45 Explain sequencing then
  - Set up a seguence table on the Chemstation
  - Print out the results in "brief" format
  - Describe what each field represents
- Does the laboratory perform a standard tune or autotune?
- 47 Describe the preventative maintenance schedule for the GC/MS and the QA/QC performed
- Would the program method used be influenced by the sample injection type?
- 49 Describe the conditions needed for using retention time data from GC/MS runs.
- Describe the use of blanks on the GC/MS.
- What conditions can influence the base peak obtained versus that of literature or reference spectrum?
- 52 Explain as to a jury how a mass spectrometer operates.

### Hands on Guide

#### MS BASICS AND HARDWARE CONFIGURATION SETTING UP ACQUISITION

Logical Troubleshooting

Functional Components of the MS

Interface Overview Vacuum Pumps

Reasons for Vacuum in a GC/MS System

Electron Ionization

How does the Quadrupole Mass Filter Work?

X-Ray Lens MS vs HED Lens MS

Define the Problem

Front Panel Checks

Views-Instrument Control Views-Data Analysis Editing an Entire Method Method Information

Inlet and Injection Parameters

Split Injections
Splitless Injections

Optimization of Split Ratios

Changing Columns and Calibration of True length

Oven Parameters

Isolation

#### **MS TUNING**

Troubleshooting Through Tuning Common Contamination Ions What does Tuning Do? PFTBA Tuning Standard Tuning Parameters Parameter Ramps

AMU Gain and AMU Gain Offset

How does AMU Gain and Offset affect Peak Widths

Mass Axis Calibration
Standard Spectra Tuning

Autotuning
Manual Tuning
Status Checks
Venting The System
Pumping Down The System
Diagnostics

### **DATA ACQUISITION**

Scan Acquisition Principles
Total Ion Chromatograms
Mass Peak Detection
Threshold
Digital Scanning Process
Spectral Tilting
SIM vs SCAN DATA

#### **QUALITATIVE DATA ANALYSIS**

General Qualitative Procedures
Standard Mouse Functions
Integration: Selecting Ions
Mass Spectral Interpretation
ChemStation Integrator
RTE Integrator
Peak Purity
ChemStation Library Searching
PBM Library Search
Parametetric Retrieval
Creating User Library

#### **QUANTITATIVE DATA ANALYSIS**

Quantitation Concepts
The Quantitation Process
Internal Standards
Setting up a Quantitation Database
Database Globes
Entering Compounds
Calibration Procedures
Quantitation Report Options
Easy ID
Q-edit

## **ULTRAVIOLET SPECTROPHOTOMETRY**

- 1. Define the following
  - Beer-Lambert Law
  - Transmittance
  - Absorbance
  - Molar absorptivity
  - Wavelength
  - Frequency
  - Electromagnetic spectrum
  - Chromophores
  - Cathode
  - Anode
  - Dynode

- What are the wavelengths of the following?
  - Visible light
  - UV
  - IR
  - Microwave
  - Radio
  - X-ray
  - Gamma rays
- What three ways can the radiation absorbed be measured and what is the formula for each?
- Is there an easy equation to remember for calculating absorbance from percentage transmittance data?
- 5 What does each component in Beer-Lambert Law stand for in A=εbc?
- 6 Below what wavelength is routine drug analysis seldom used for UV?
- Why is it generally preferable to use absorbance as a measure of absorption rather than % Transmittance?
- 8 Does a compound with a high molar absorptivity have a higher or lower limit of detection than a compound with low molar absorptivity?
- 9 Does the solvent in which the absorbing species is dissolved affect the spectrum of the species?
- 10 What is charge-transfer absorption?
- 11 Draw the schematic diagram of a double-beam UV/Vis spectrophotometer and name the parts.
- What types of lamps are used for UV/Vis radiation?
- 13 Which type of lamps are used on our instruments?
- Why are guartz window and cuvettes used for UV/Vis analysis?
- Why is it important that the radiation source does not change abruptly over its wavelength range?
- 16 What component parts make up a monochromator?
- 17 What type of detector is commonly used in UV/VIS spectroscopy?
- What do you need to know to calculate the percentage of base in the below drugs? And where would you find the values needed.
  - Cocaine
  - Heroin
  - Methamphetamine

## **FTIR**

- What is infrared spectrophotometry? Describe the theory behind its use as an identification technique including types of information obtained and specificity.
- 2 Draw a schematic diagram for a double-beam IR.
- 3 Describe the electromagnetic spectrum.
- 4 What is the upper and lower limit on the infrared region of the electromagnetic spectrum?
- 5 What region is the most useful analytically?

- What is the standard range of most instruments?
- 7 Define the following
  - Wavelength
  - Wavenumber
  - Frequency
  - Dipole moment
  - Absorption
  - Transmittance
  - Harmonic vibration
  - Combination band
  - Fundamental vibration
  - Monochromator
  - Interferometer
  - Amplitude
- 8 Draw a block diagram of the FTIR and describe the function of the major components.
- 9 Describe the different types of radiation sources for FTIR instruments.
- 10 Describe the different types of detectors available for FTIR instruments.
- 11 What is "Fourier Transform" and how does it apply to IR?
- 12 Explain the theory behind the Attenuated Total Reflectance (ATR) sampling unit.
- Describe the differences in the spectra obtained using ATR versus regular transmittance.
- 14 Explain the function of the ATR correction within the software.
- 15 Is this spectrum permissible to use in case work?
- What is meant by the "fingerprint region" of an IR spectrum? Why is it significant?
- 17 Can IR differentiate optical isomers? Diastereomers? Structural isomers?
- 18 Why is polystyrene used to check the function of the FTIR?
- 19 Which organic functional groups correspond to the following absorption frequencies?
  - 3639-3633 cm<sup>-1</sup>
  - 2990-2850 cm<sup>-1</sup>
  - 1650-1510 cm<sup>-1</sup>
  - 1750-1740 cm<sup>-1</sup>
  - 770-690 cm<sup>-1</sup>
  - 760-540 cm<sup>-1</sup>
- 20 What two conditions must be met in order for infrared absorption to occur?
- 21 What is the intensity of an IR absorption proportional to?
- What are the two basic categories of molecular vibration?
- What are the four types of bending?
- What is meant by vibrational coupling?
- 25 Describe the differences between dispersive and non-dispersive instruments.
- What are the advantages of FTIR over dispersive IR?
- 27 Which will vibrate with higher frequency, C-H bond or a C-C bond and why?

- 28 What does hydrogen bonding do to the vibrational frequency of a hydroxyl or an amine group?
- 29 Describe the absorptions range for the following groups:
  - -0-H
  - -N-H
  - >C=O
  - -C-O-
  - –C–H
  - –C≡N
  - –NO<sub>2</sub>
  - Aromatic substitutions
- What is polymorphism and how does it influence IR spectra?
- 31 What model IR does our laboratory use?
- What radiation sources and detectors are used in the FTIR and its attachments in our laboratory?
- What problems are encountered in using IR as a quantitative technique?
- What causes a sloped baseline?
- 35 Explain baseline correction and how it is performed and why.
- What is spectral subtraction and under what conditions is it use?
- What are the differences between background subtraction and spectral subtraction?
- What resolution are samples normally run in your laboratory?
- What computer libraries are available in your lab and what are the resolutions of the spectra contained in them?
- Describe how a spectrum is auto-saved and/or saved.
- 42 Describe how ATR analysis can be run on powders, liquids, and mixtures.
- What are the advantages/disadvantages of a GC/MS compared to an IR when used for identification purposes?
- Describe the preventative maintenance schedule and the QA/QC procedures performed on the IR, including the VAL-Pro software.
- Describe, as to a jury, how an FTIR operates.