



TOXTALK

Society of Forensic Toxicologists, Inc.

1013 THREE MILE DRIVE • GROSSE POINTE PARK • MICHIGAN 48230-1412

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1989 MEETING HOST

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I would like to take this opportunity to thank Joseph A. Crifasi for the enclosed technical article on the elimination/generation of mass spectrometry base peaks and the related macro for H.P. users. The article was submitted some time ago, but dissemination of other information on a timely basis has prevented its appearance until this issue. I am sure you will find the article useful. Remember, this is the third article appearing in ToxTalk relative to this topic.

You are invited to submit technical articles for consideration to ToxTalk. The procedure is simple and described at the bottom of this page. There is a wealth of information available among SOFT members - share a little!

The Laboratory Guidelines Committee met as scheduled in Chicago on Friday, April 21st, through Sunday, April 23rd. All 11 committee members were present, and a very productive meeting resulted. The "Draft Report" as circulated in the last issue of ToxTalk was reviewed and revised, and further assignments were given by Chairman Michael Peat. The next meeting of the committee in its entirety is scheduled the weekend of July 28-30, utilizing the Friday through Sunday format. With another productive session, this committee will be one step closer to the generation of a quality product useful to practicing forensic toxicologists. A full report will be presented at the SOFT annual meeting in Chicago in October.

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TECHNICAL HIGHLIGHTS: ALTERING MASS SPECTRUM BASE PEAKS
BY JOSEPH A. CRIFASI

OF SPECIAL INTEREST: 1989 SOFT MEETING INFORMATION

INSERTS: CALL FOR PAPERS - DUES NOTICE

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ToxTalk is mailed quarterly to members of the Society of Forensic Toxicologists, Inc. For membership information contact: Richard D. Pinder, Ph.D., SOFT Secretary, Office of the Chief Medical Examiner, 11 Shuttle Road, Farmington, CT 06032 telephone: (203) 679-3980

All members and others are invited to contribute to ToxTalk. Submit all materials (original plus 3 copies, if possible) for publication consideration to: ToxTalk, 1013 Three Mile Drive, Grosse Pointe Park, Mi 48230-1412.
DEADLINES: February 1, May 1, August 1, and November 1.

* * * NEXT TOXTALK DEADLINE: AUGUST 1, 1989 * * *

PLANS FOR EXCITING 1989 S.O.F.T. MEETING UNDERWAY
OCTOBER 18-21 **CHICAGO (Ambassador West Hotel)**

Dr. Michael Schaffer, 1989 SOFT Meeting Host, offers the following tentative schedule. The information is subject to change (i.e. number of papers submitted, etc. will determine final schedule).

WEDNESDAY: October 18, 1989

- 2:00 - 5:00 WORKSHOP: CLINICAL "FORENSIC" TOXICOLOGY, i.e., Clinical Toxicology for the Forensic Toxicologist (Daniel Hryhorczuk, M.D., Chief, Section of Toxicology and Dept. of Occupational Medicine, Cook County Hosp., and Eleanor Berman, Ph.D. - Chief, Toxicology Dept., Cook County Hosp. Lab). Topics include: Toxic Alcohols, Organic Solvents, Asphyxiant Gases, Cocaine, Arsenic, and Analgesics.
- 5:00 - 7:00 AMBASSADOR WEST COCKTAIL RECEPTION - *hospitality exclusively for SOFT meeting attendees registered at the Ambassador West Hotel
- 7:00 - 9:00 SOFT WELCOME RECEPTION - for all meeting registrants

THURSDAY: October 19, 1989

- 9:00 a.m. OPENING REMARKS - R. J. Stein, M.D., Medical Examiner, Cook County
- 9:10 - noon SCIENTIFIC SESSION - Platform Presentations
- noon - 1:30 LUNCHEON SEMINAR - "MONITORING THE ENVIRONMENT FOR TOXIC EXPOSURE" (Naresh Jain, Ph.D. and Tom Sneath, B.S.)
- 2:00 - 4:00 SCIENTIFIC SESSION - Platform Presentations featuring papers in The areas of Clinical "Forensic Toxicology," Environmental Toxicology and other areas of interest
- 4:00 - 5:00 POSTER SESSION
- 5:00 - 7:00 AMBASSADOR WEST COCKTAIL RECEPTION - *SOFT hotel guests only

FRIDAY: October 20, 1989

- 9:00 - noon SCIENTIFIC SESSION - Platform Presentations
- noon - 2:00 SOFT AWARDS BANQUET (included in registration fee)
- 2:00 - 4:00 GC/MS FORENSIC SYMPOSIUM Moderator - Nancy Wu Chen, Ph.D., Participants - John Cody, Ph.D., Roger Foltz, Ph.D., James Garriott, Ph.D., Michael Peat, Ph.D., and Michael Schaffer, Ph.D. Topics to be discussed: Instrument Performance Evaluation; Standards and Controls, QC Documentation; Full Scann -vs- SIM; Criteria of Identification; Quantitation; Common Problems.
- 4:00 - 5:00 POSTER SESSION
- 5:00 - 7:00 AMBASSADOR WEST COCKTAIL RECEPTION - *SOFT hotel guests only
- evening PRESIDENT'S INFORMAL CONFERENCE

SATURDAY: October 21, 1989

9:00 - 10:30 LABORATORY GUIDELINES COMMITTEE REPORT. Michael Peat, Ph.D.,
(Chairman) and committee members

10:30 - noon SOFT ANNUAL BUSINESS MEETING

2:00 - 5:00 WORKSHOP - DRUG USE TESTING: FOCUS ON INTERPRETATION OF RESULTS.
Moderator Kurt Dubowski, Ph.D.; guest speakers will be announced.

The following information is offered as a guide to help you plan for this meeting. Exact information will be provided in a separate mailing scheduled for August 1st. Of course, further information will be published in the September issue of ToxTalk.

HOTEL: The Ambassador West is a beautifully-appointed hotel within easy walking distance of magnificent shopping and a variety of restaurants. Hotel accommodations can be difficult in Chicago so be sure to reserve early - hotel reservation deadline is October 2nd - reservation cards will be in the August mailing. SOFT has been given a discounted rate of \$118 (does not include taxes) per single room. If you are familiar with Chicago hotel rates, you will recognize a significant discount. This reduced rate will be applied to Saturday night as well if you choose to stay over until Sunday.

AIR FARE: United Airlines is offering a discount on all fares to Chicago for anyone participating in the SOFT meeting. Don't forget a tremendous savings can sometimes be realized by departing Chicago on Sunday. Instructions will appear in the special August mailing.

REGISTRATION FEES: SOFT members and persons who submit completed membership applications before July 1st are eligible for reduced fees. The following fees are reliable but not definite and noted to help you budget for the meeting.

SOFT MBR/APPL NON-MBR

\$45	\$85	SOFT MEETING REGISTRATION (includes Welcome Reception and Awards Banquet)
\$15	\$15	LATE FEE (register after September 27th)
\$10	\$10	Extra reception ticket 10/18
\$25	\$25	Extra Awards Banquet ticket 10/20
\$35	\$50	10/18 WORKSHOP: Clinical "Forensic" Toxicology
\$20	\$25	10/19 LUNCHEON SEMINAR: "Monitoring the Environment for Toxic Exposure"
\$50	\$75	10/21 WORKSHOP: "Drug Use Testing - Focus on Interpretation of Results"

CORPORATE SPONSORS: The following companies will be exhibiting at the 1989 SOFT meeting: Roche Diagnostic Systems, Hewlett Packard Co., Abbott Diagnostics, JAT/Preston Publications, Diagnostic Products Corp., Sigma Chemical Co., Supelco, Inc., Finnigan MAT, Radian Corp., Toxi-Lab, Inc., and Dynatech Laboratories, Inc. Only one additional exhibit space may possibly be available. Sponsors for workshops and coffee breaks and program advertisers are welcome. Corporate sponsors will be properly acknowledged. We value your continued support.

For further information contact: SOFT MEETING INFORMATION, 1013 Three Mile Dr., Grosse Pointe Park, MI 48230-1412 (313-884-4718). non-members who have already contacted SOFT will automatically receive meeting information.

ALTERING MASS SPECTRUM BASE PEAKS

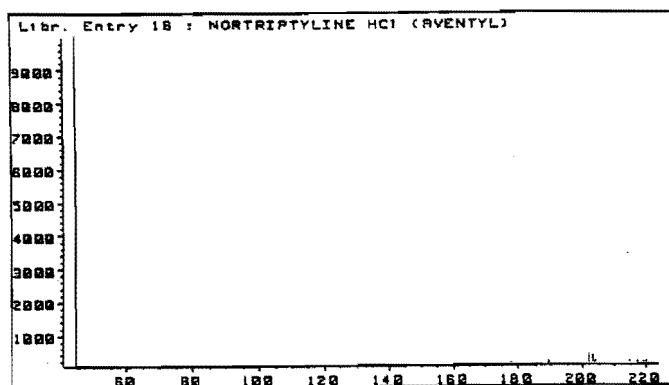
Submitted by: Joseph A. Crifasi, M.S., M.T. (ASCP), Memorial Medical Center, Toxicology Laboratory, Springfield, IL.

Several articles have appeared in ToxTalk regarding the elimination of mass spectrometry base peaks to distinguish between drugs which have similar mass spectra. This is particularly helpful in instances where drugs have a dominant base peak without additional ion fragments of substantial abundance.

Since past articles have dealt with mass spectra having a dominant 58 base peak, it should be emphasized that the technique of removing base peaks can also be useful for other drugs, such as those with virtually only a base peak of 44. Examples are shown in Figures 1 and 2.

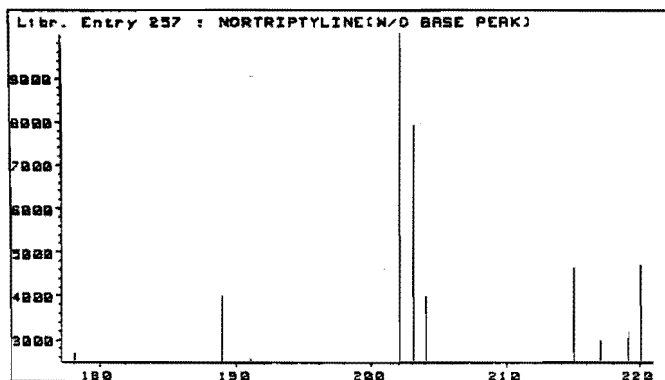
A macro program may be used to alter the original mass spectrum of a drug, generate a new spectrum, and perform a library search which displays the match quality (Figure 3). The macro program uses stored data files which contain mass spectral scans of drugs from 45 to 60 AMU and 30 to 45 for use with base peaks of 58 or 44, respectively. The necessary data file is entered by name into the macro program. The retention time for the peak to be used must be entered, as well as the library file name (Figure 4). This macro program may be useful to 5970B MSD users with the 59970B chemstation.

FIGURE 1: Mass spectra of drugs with dominant 44 base peak before and after removal (nortriptyline)



Libr. Entry 16 : NORTRIPTYLINE HCl (AVENTYL)
MEMORIAL MEDICAL CTR TOXICOLOGY DATABASE

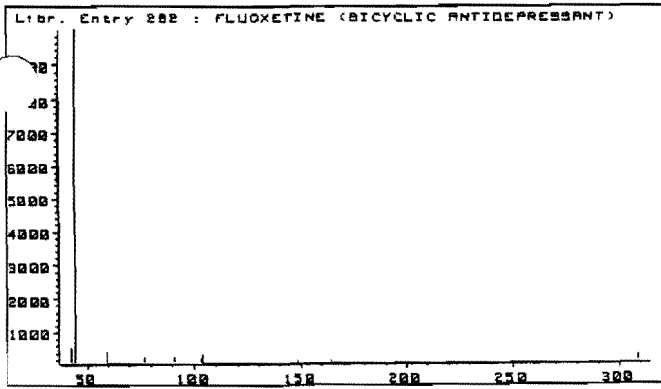
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.05	9999	201.95	357	214.95	162	219.05	99
178.00	110	202.95	295	217.05	104	220.05	151
189.00	155	203.95	142				



Libr. Entry 257 : NORTRIPTYLINE(W/O BASE PEAK)
MEMORIAL MEDICAL CTR TOXICOLOGY DATABASE

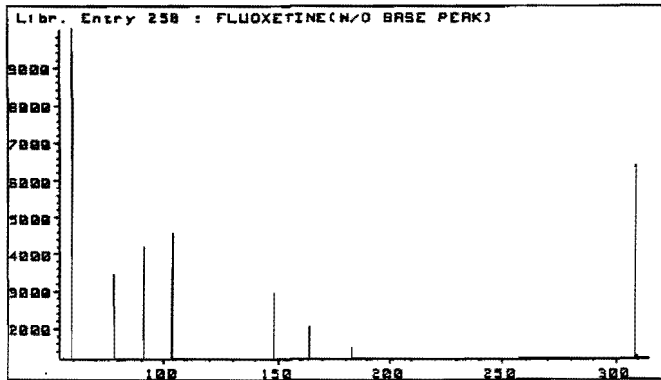
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
178.10	2690	202.10	9999	215.00	4611	219.10	3031
189.00	3972	203.10	7880	217.00	2965	220.10	4660
191.10	2518	204.10	3961				

FIGURE 2: Mass spectra of drugs with dominant 44 base peak before and after removal (fluoxetine)



Libr. Entry 262 : FLUOXETINE (BICYCLIC ANTIDEPRESSANT)
MEMORIAL MEDICAL CTR TOXICOLOGY DATABASE

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.10	507	77.05	235	104.10	321	164.10	109
44.10	9999	91.10	250	148.10	143	309.15	274
59.05	381	103.10	203				



Libr. Entry 258 : FLUOXETINE(W/O BASE PEAK)
MEMORIAL MEDICAL CTR TOXICOLOGY DATABASE

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
59.05	9999	103.05	2717	164.10	2047	309.10	6379
78.05	3404	104.05	4557	183.10	1474	310.10	1236
91.05	4168	148.05	2941				

FIGURE 3: Macro program printout of library search results after removal of base peak.

LIBRARY SEARCH RESULTS

Scan 527 (12.495 min) of NORT.D

Library file: MMC.L

Library name: MEMORIAL MEDICAL CTR TOXICOLOGY DATABASE

	CAS #	Library Index #	Match Quality
1: NORTRIPTYLINE(W/O BASE PEAK)	894713	257	9993
2: AMITRIPTYLINE(W/O BASE PEAK)	549188	256	8723
3: CYCLOBENZAPRINE(W/O BASE PEAK)	6202239	260	5055
4: DESMETHYLDOXEPIN(W/O BASE PEAK)	0	255	4868
5: DOXEPIN(W/O BASE PEAK)	1229294	254	4754
6: CHLORPHENIRAMINE MALEATE(CHLOR-TRIMETON)	113928	84	4333
7: PENTAZOCINE HCl (TALWIN)	2276520	74	3177
8: NOSCAPINE (NARCOTINE)	128621	236	3056
9: PROTRIPTYLINE HCl (VIVACTIL)	1225554	17	2587
10: NORPROPOXYPHENE(W/O BASE PEAK)	0	253	2321

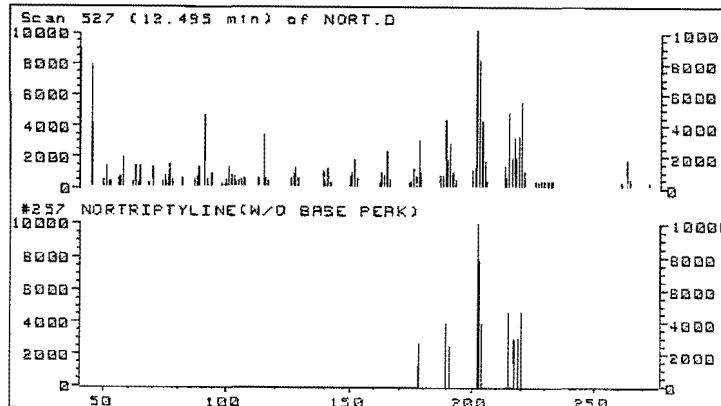


FIGURE 4: Macro programs for removing 58 and 44 base peaks.

```
NAME REMOVE58
CLEAR
FILE
TIC
EX X,Z
CLEAR
DR 3,Z
MESS "SELECT PEAK TO CONFIRM      ",,18,3
CURSOR
SPECTRUM(X)
FI 58.D ← Enter Data File for 45 to 60 amu scan.
CLEAR
TIC
EX Z,X
SP(7.555) ← Enter retention time for peak with 58 ion.
EX Z,Y
SUB SUPPRESS
NORM
DR 3,X
SEARCH MMC.L ← Enter your library file name here.
TAB RESULTS, PRINTER:
RET 1
MERGE
DR 3,X
GRAPHICSCOPY
CLEAR
FIRSTTIME=0
```

```
NAME REMOVE44
CLEAR
FILE
TIC
EX X,Z
CLEAR
DR 3,Z
MESS "SELECT PEAK TO CONFIRM      ",,18,3
CURSOR
SPECTRUM(X)
FI 44.D ← Enter Data File for 30 to 45 amu scan.
CLEAR
TIC
EX Z,X
SP(10.157) ← Enter retention time for peak with 44 ion.
EX Z,Y
SUB SUPPRESS
NORM
DR 3,X
SEARCH MMC.L ← Enter your library file name here.
TAB RESULTS, PRINTER:
RET 1
MERGE
DR 3,X
GRAPHICSCOPY
CLEAR
FIRSTTIME=0
```

THE JOURNAL CLUB

Submitted by: H. Chip Walls, Forensic Sciences, 1826 Cedar Crest Road, Birmingham, AL 35214

is the intent of this on-going feature to call attention to unusual or highly interesting articles, not a systematic review of selected journals such as available through other recognized sources. Citations 1-28 appeared in earlier issues of ToxTalk. You are encouraged to send contributions for this column to ToxTalk. Be sure to include proper citation or source address/telephone number.

(29) MECHANISMS OF DEPRESSANT DRUG ACTION/INTERACTION. Recent Dev Alcohol #4:39-60, 1986.

(30) FREE DRUG MONITORING. Clin Lab Med 7(2):279-287, 1987.

(31) FREE DRUG MONITORING IN CLINICAL PRACTICE: RATIONALE AND CURRENT STATUS. Pharmacokinet 11(6):50-69, 1986.

(32) DRUG BINDING TO HUMAN ALPHA-1-ACID GLYCOPROTEIN IN HEALTH AND DISEASE. Pharm Reviews 40(1):1-36.

The articles above cover clinical protein binding for starters.

(33) COCAINE: REVIEW OF THE CURRENT LITERATURE AND INTERFACE WITH THE LAW. Behavioral Sci and the Law 3(3):283-298, 1985.

(34) PHENCYCLIDINE AND VIOLENCE: CLINICAL AND LEGAL ISSUES. J Clin Psychopharm 8(6):397.

(35) TOXIC PSYCHOSIS: Modern Perspectives in Clinical Psychiatry. Chapter 12, p231. Have you been exposed to the defense of "cocaine or drug induced psychosis?" Psychiatry has the answer!

(36) A great source for drug information and "pill" description is the USP-DI Vol #3. For those who have access to a poison control center, use their POISONDEX, a clinically-oriented device but full of "neat information."

(37) CLINICAL PHARMACOKINETICS OF NON-OPIATE ABUSED DRUGS. Clin Pharmacokinetics 16:1-26, 1989.

(38) ANALYTICAL PROFILES OF SUBSTITUTED 3,4-MDA'S: DESIGNER DRUGS RELATED TO MDA. Order from CND Analytical, P.O. Box 1527, Auburn, ALA 36831-1527 (\$35.00).

(39) REDUCED TCA LEVELS DUE TO GEL SEPARATORS. J Clin Psycho 17(6):423-4.

(40) EFFECTS OF BLOOD COLLECTION TUBES ON ANTIDEPRESSANT CONCENTRATIONS J Chrom 423:373-5, 1987.

Could #39 and #40 be another postmortem re-distribution problem?

(41) MODERN SCREENING STRATEGIES IN ANALYTICAL TOXICOLOGY WITH SPECIAL REGARD TO NEW BENZODIAZEPINES. Rechtsmed 100(1):19-37, 1988. This has answers to a lot of the triazolobenzos and data for a screening program which can be used with Toxi-Lab data.

(42) VALIDITY OF POST MORTEM CHEST CAVITY BLOOD ETOH DETERMINATIONS. J Chrom 449(1):337-40. Just when we "convince" pathologists not to scoop blood from the chest cavity!

(43) DETECTION OF BENZODIAZEPINES IN FORENSIC SCIENCE INTEREST... J Chrom 449(1):281-297. Another solid phase extraction and blood protein binding consideration.

(44) RADIOIMMUNOASSAY OF DRUGS IN BODY FLUIDS IN A FORENSIC CONTEXT. For Sci Prog 3:1-89.

(45) ANALYSIS OF DRUG POSITIVE BLOOD SAMPLES AFTER STORAGE. Beit Gerichtl Med 46:95-101, 1988.

* * * * *

Nominating Committee 1990 Slate to appear in the next issue of ToxTalk

HAVE YOU PAID YOUR
1989-90 S.O.F.T. DUES??

ELMER GORDON OPEN FORUM

Chip Walls would like to know if anyone has seen the use of TAC solution in E.R. patients who become morgue cases (tetracaine 0.5%, cocaine 10%, adrenalin). See JOURNAL CLUB.

NIPPLE TUBE SUPPLIER NEEDED: Former supplier out of business (Laboratory Research Co., concentratubes, flint glass, 114x18 mm, \$25/100). If you have a supplier, please contact Joan Vogel, Westchester County, Dept. of Laboratories & Research, Valhalla, NY 10595 (telephone: 914-347-6169).

DIRECTORY UPDATE

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Richard N. Phillips, Ph.D., Baxter - Dade Division, P.O. Box 520672, MS 390, Miami, FL 33152-0672

Be sure to inform Secretary Pinder (address on page one) of any change in your address so you can get the latest SOFT news!

TREASURY NOTES

Treasurer Lewis would like to remind you that the current fiscal year ends June 30, 1989. If you require reimbursement for any expenses, please submit your request to Mark Lewis before June 30th. And don't forget to pay your 1989-90 SOFT dues.

PROFESSIONAL CALENDAR

CALIFORNIA ASSOCIATION OF TOXICOLOGISTS 1989 quarterly meetings: Aug 5 - Northern California; Nov. 4 - San Diego, CA. For further meeting and workshop information, please contact Lee B. Knight, CAT Vice President, Memorial Healthtech Laboratories, 701 E. 28th St., Suite 113, Long Beach, CA 90806 (telephone: 213-595-3427).

S.O.F.T. ANNUAL MEETING: Oct. 18-21, 1989, Ambassador West Hotel, Chicago, IL. Preliminary plans include plenary sessions, breakfast & luncheon seminars, Wednesday & Saturday workshops and the customary SOFT activities. See related article in this issue of ToxTalk. For further information, contact SOFT Admini. Office, 1013 Three Mile Drive, Grosse Pointe Park, MI 48230-1412 (313) 884-4718 or 1989 SOFT Meeting Host Michael Schaffer, Ph.D., Cook County M.E.O., 2121 West Harrison Street, Chicago, IL 60612 (telephone: 312-666-0500).

11th INTERNATIONAL CONFERENCE ON ALCOHOL, DRUGS AND TRAFFIC SAFETY: October 24-27, 1989, Ambassador West Hotel, Chicago, IL. Program includes a keynote speaker, invited speakers for the plenary session followed by responders, concurrent sessions for the presentation of papers, poster sessions and exhibitors. For further information contact Al Lauersdorf, T-89 Secretary, National Safety Council, 444 N. Michigan Avenue, Chicago, IL 60611 (telephone: 312-527-4800).

November 1989: PAN AMERICAN ASSOC. OF FORENSIC SCIENCES, Bogota, Colombia. Theme: "The Sciences and Justice." Contact: President Dr. Egon Lichtenberger, Carrera 11 A 96-26, Bogota, Colombia.

Future SOFT meeting sites: 1989 - Chicago, IL (Michael Schaffer, Ph.D)
1990 - New York City area (Michael McGee)
1991 - Canada (joint meeting with CSFS)
1992 - Connecticut
1993 - Joint meeting with CAT
1994 - Atlanta, GA



SOCIETY OF FORENSIC TOXICOLOGISTS, INC.
ABSTRACT OF PAPER FOR 1989 ANNUAL MEETING
OCTOBER 18-21, 1989 CHICAGO, ILLINOIS

NAME AND ADDRESS OF PRESENTING AUTHOR

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IS PRESENTING AUTHOR A SOFT MEMBER?

YES _____ NO _____

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ABSTRACT DEADLINE: JUNE 30, 1989

1. PLEASE DESCRIBE METHODS, ANALYTICAL RESULTS WITH DISCUSSION OF THE DATA IN THE ABSTRACT.
2. PLEASE SUMMARIZE YOUR CONCLUSIONS OR RESULTS IN THE ABSTRACT.

3. SIGNATURE OF SUBMITTING AUTHOR:

4. THE ABSTRACT REVIEW COMMITTEE RESERVES THE RIGHT OF FINAL PLACEMENT OF THE PRESENTATION IN EITHER PLATFORM OR POSTER SESSION.





1989-90 DUES NOTICE

YOUR DUES FOR THE 1989-90 MEMBERSHIP YEAR IN THE SOCIETY OF FORENSIC TOXICOLOGISTS, INC. ARE DUE. PLEASE COMPLETE BELOW AND RETURN THE BOTTOM PORTION WITH A CHECK PAYABLE TO S.O.F.T., INC. TO:

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DEADLINE: JUNE 30, 1989 REMEMBER, THE SOFT FISCAL YEAR IS JULY 1, 1989 TO JUNE 30, 1990. IF YOUR DUES ARE NOT PAID BY JULY 1ST, YOU WILL BE CONSIDERED IN ARREARS.

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___ RETIRED

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ERA CONTRIBUTION \$ _____

TOTAL ENCLOSED \$ _____

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