NEIC

EPA-330/9/80-003

NEIC COMPUTER ASSISTED EVALUATION OF GC/MS DATA

For Organic Priority Pollutant Analysis And Organic Characterization

October 1980

EPA

national enforcement investigations center

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UNITED STATES ENVIRONMENTAL PROTECTION

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NATIONAL ENFORCEMENT INVESTIGATIONS CENTER
Denver, Colorado

CONTENTS

1.0 INTRODUCTION

1.1 The report describes an automated procedure developed at NEIC for evaluating GC/MS data collected using standard analytical methods. The procedure generates quantitative data for preselected compounds, and it can optionally generate qualitative GC/MS characterization of other organic compounds that are present in a sample.

2.0 SUMMARY OF METHOD

2.1 The automated procedure EVALØ processes a data file by locating an internal standard (IS) within a fixed retention time (RT) window, and by locating preselected or target compounds within fixed relative retention time (RRT) windows. One internal standard is used for quantitative measurement and relative retention time calculation. One or more internal standard may be used for quality assurance of GC/MS operating conditions and of standard analytical methods. Target compounds (compounds of interest) are located in the data file and identified using relative retention time data and a computerized reverse-search library procedures. In reverse search, the mass spectrum of a target compound is selected from a user-created library of standard reference compounds and compared to mass spectra in the GC/MS run within a set relative retention time window. If the compound is located in the GC/MS run, the area of preselected ion is measured and stored. The procedure prints a copy of the reconstructed ion chromatogram (RIC), the mass spectrum of each target compound detected, and the quantitation and identification report for each file processed. The identification report indicates how well the library spectrum of a target compound matches the sample compound spectrum. Compounds other than target compounds (unknowns) present in the sample can be compared to the entries in the National Bureau of Standards (NBS) library of mass spectra. If the analyst elects to identify unknown compounds in the sample, the procedure prints a comparison of unknown spectra to library spectra, and a qualitative report listing its best identification of unknown compounds.

3.0 INTERFERENCES

3.1 A compound may meet identification criteria and not be quantitated because the ion preselected for quantitation was not intense enough in the run. When a target compound is not quantitated, a "NOT FOUND" is printed in the quantitation report.

3.2 Multiple entries for a single compound may be printed in the quantitation list. Multiple identifications may occur when the ions used to identify a compound maximize more than once within the relative retention time window set for that compound. Extraneous entries are deleted after manual evaluation of the mass spectra by the analyst.

3.3 If chemical isomers elute close to one another, the procedure may mislabel the compounds. Manual examination of the mass spectra and the RIC usually results in the correct identification and quantitation of the compounds. A few isomers are reported as isomer pairs.

4.0 APPARATUS AND PERSONNEL

4.1 The user procedures were assembled on Finnigan INCOS software, Revision 3.1 and compatible hardware.

4.2 Personnel must know how to use Finnigan INCOS software. The person(s) must have a working knowledge of procedure writing and execution, the awareness to differentiate a software problem from a hardware problem, and the ability to solve or circumvent a software problem.

5.0 PROCEDURE

5.1 Start Up

1. Load the procedures, methods, library lists, and the user library listed in Appendix A onto the INCOS system disc.

2. Examine chromatograms of standard reference compounds. Locate and identify all of the standard compounds. Record the scan number of the internal standard used for quantitation and relative retention time calculation. (Each standard reference mixture or sample must contain at least one internal standard.) Calculate the RRT for each standard reference compound using a routine available in the data system.

3. Study the mass spectrum of each standard. Select an ion that is characteristic of the compound. The ion that is most often chosen is the most intense ion or base peak. The ion selected for any compound must be different in mass from the ion chosen for the compound that elutes directly before it or immediately after it in the chromatographic run. If the selected ion is not the base peak, it must be at least 50% as intense as the base peak.

4. Create a user library containing the mass spectra of interest (target compounds). Each library entry should contain, in addition to mass and intensity data, relative retention time (RRT), quantitation mass (ion used for quantitation), standard amount, reference peak (internal standard).

5. Evaluate standard reference mixtures using the automated prescreening procedure (EVALØQ or ESETØ). Check the resulting quantitation list to be certain that all of the compounds in the standard mix are present. If a compound is not present, locate the peak manually and add its area to the quantitation list.

6. Execute the master evaluation procedure (EVALØ). If all of the standard components are found, use the data system to update response factors, retention times, and relative retention times. If all of the standard reference components are found, an audit has already been performed by the master evaluation procedure on the standard retention times and relative retention times.

7. Audit the standard compound response factors using procedure RFQUAL.

8. The data system has now been standardized. It is ready to evaluate daily standards, samples, and quality control samples.

5.2 Routine Operation

1. Analyze standards. Once the data system has been standardized (as in Section 5.1), daily standards must be run to ascertain if the instrument is operating within the quality assurance limits set by the analytical procedure.

2. Evaluate standards using the master evaluation procedure (EVALØ). Update the retention times, relative retention times, and response factors for each compound. Updating the standard parameters permits a correction for small daily variation in instrument response. A copy of the daily standardization factors must be kept with the sample(s).

3. Append the response factor for each standard compound to a response list for that compound. Determine if the daily standard response factors are within the limits set by the analytical method using procedure RFQUAL.

4. Analyze samples and quality control samples using the same instrument conditions used to analyze standards. Quality control samples include blanks, replicates, and spikes.

5. Evaluate samples using the master evaluation procedure (EVALØ). The procedure will locate and quantitate target compounds using the standard parameters stored in the system. The analyst can elect to have the procedure identify non-target organic compounds that are present.

6.0 QUALITY CONTROL

6.1 The analytical instrument is calibrated to meet the specifications described in the analytical method.

6.2 The daily standardization of the analytical instrument includes blank analyses and standard reference mixture analysis. A daily standard analysis permits the analyst to update quantitation parameters prior to sample analysis. The daily retention times and relative retention times are audited by the master evaluation procedure EVALØ. The daily response factors are audited by the procedure RFQUAL. The daily retention times, relative retention times, and response factors should not vary beyond the limits set by the analytical method. If these parameters do exceed the limits, the standard analysis should be rejected and rerun.

6.3 One internal standard is added to the sample or sample mixture prior to GC/MS analysis. This internal standard is used for relative retention time calculations and for quantitative measurement of sample components. One or more internal standard may be added to the sample for quality assurance of GC/MS operating conditions and of standard analytical methods.

6.4 The mass chromatogram of the internal standard(s) is examined to check the peak shape of the ion used for quantitation for any abnormalities such as the splitting of the peak, and to monitor the area of the peak(s). The procedure ISCHK locates and quantitates the internal standard compound(s) in standard mixture analyses and in sample analyses. The operator records these area values and computes the experimental limits of the values. If the peak area of the internal standard(s) exceeds the experimental limits established by the operator, the standard run or the sample run must be rejected.

6.5 Each compound identification is audited by manual examination of the mass spectrum. The identity of a compound is confirmed: (a) if its relative retention time agrees with that of a standard analyzed under identical conditions to within ± 10%, (b) if three characteristic ions maximize in the spectrum, and (c) if the ratios of the intensities (peak height) of these three ions agree within ± 20% to those ratios in a standard reference compound.

6.6 The accuracy of the quantitative measurements is monitored with the aid of replicate analyses and the addition of spiking solutions.

7.0 PRECISION AND ACCURACY

7.1 The overall precision and accuracy is limited by the quality of the raw data evaluated.

8.0 REFERENCES

(1) "Green List: Recommended List of Priority Pollutants", April 1977, Revised.

(2) "Sampling and Analysis Procedures for Screening of Industrial Effluents for Priority Pollutants", U.S. EPA, Environmental Monitoring and Support Laboratory, Cincinnati, Ohio, March 1977, Revised April 1977.

(3) "INCOS Data System - MSDS Operators Manual - Revision 3", Finnigan Instruments, March 1978.

(4) "Quality Assurance Program for the Analyses of Chemical Constituents in Environmental Samples", U.S. EPA, Environmental Monitoring and Support Laboratory, Cincinnati, Ohio, March 1978.

(5) "Organic Pollutant Analysis Quality Assurance and Document Control Procedures", U.S. EPA, NEIC, Denver, Colorado, Revision 1, April 1979.

(6) "Part III Environmental Protection Agency Guidelines Establishing Test Procedures for the Analysis of Pollutants; Proposed Rules", Federal Register, Vol. 44, No. 233, Monday, December 3, 1979. Washington, D.C.: U.S. Government Printing Office.

APPENDIX A

Procedures, Methods, Library Lists, and User Library Associated with Automated Evaluation of GC/MS Data

Base/Neutral Library List

Volatiles in Air Library List

Acid Library List

Volatiles in Water Library List

Priority Pollutant Library List

EVALØ.PR
EVALØA.PR
EVALØB.PR
EVALØC.PR
EVALØD.PR
EVALØE.PR
EVALØF.PR
EVALØG.PR
EVALØH.PR
EVALØI.PR
EVALØJ.PR
EVALØK.PR
EVALMØ.PR
EVALM1.PR
EVALM2.PR
PRINP1.ME
PRINP2.ME
PRINNM.ME

EVAL2.PR
EVAL2A.PR
EVAL2B.PR
EVAL2C.PR
EVAL2D.PR
EVAL2E.PR
EVAL2F.PR
EVAL2G.PR
EVAL2H.PR
EVAL2I.PR
EVAL2J.PR
EVAL2K.PR
EVALMØ.PR
EVALM1.PR
EVALM2.PR
PRINP1.ME
PRINP2.ME
PRINNM.ME

ESPEC.PR
ESPEC1.PR
ESPEC2.PR
ESPEC3.PR
ESPEC4.PR
ESPEC5.PR
ESPEC6.PR
ESPEC7.PR
PRINE1.ME
PRINE2.ME
PRINNM.ME

ISCHK.PR
ISCHK1.PR

MQIS.PR

ESETØ.PR
ESETA.PR

ESET2.PR
ESETA.PR

EVALØQ.PR
EVALØC.PR
EVALØD.PR
EVALØF.PR
EVALØG.PR
EVALØH.PR
EVALØI.PR
PRINP2.ME

EVAL2Q.PR
EVAL2C.PR
EVAL2D.PR
EVAL2F.PR
EVAL2G.PR
EVAL2H.PR
EVAL2I.PR
PRINP2.ME

MQSA.PR

RFQUAL.PR
RFQC.MS
RFQC.IN

EVALSP.PR
EVALS1.PR

EVALLB.PR
EVALL1.PR

DISK.PR
DISK1.PR
DISK2.PR
LOG.MS
LOG.IN

ACCHK.LL
BNCHK.LL
VOLCHK.LL
AIRCHK.LL

PPBN.LL
PPVOL.LL
PPPH.LL
PPAIR.LL
PP.LL
LibraryPP.LS
LibraryPP.LX

INPUT FILE	PPBN LL,	OUTPUT FILE	PPBN LL						
PP, 129	PP, 1	PP, 5	PP, 8	PP, 9	PP, 12				
PP, 18	PP, 20	PP, 25	PP, 26	PP, 27	PP, 28				
PP, 35	PP, 36	PP, 37	PP, 39	PP, 40	PP, 41				
PP, 42	PP, 43	PP, 52	PP, 53	PP, 54	PP, 55				
PP, 56	PP, 62	PP, 63	PP, 66	PP, 67	PP, 68				
PP, 69	PP, 70	PP, 71	PP, 72	PP, 73	PP, 74				
PP, 75	PP, 76	PP, 77	PP, 78	PP, 80	PP, 81				
PP, 84	PP, 130	PP, 136							

NAM	NUM	WT	FORMULA	NAME
PP	129	212	C16 D10	ISB D10-PYRENE (129)
PP	1	154	C12 H10	01 ACENAPHTHENE
PP	5	184	C12 H12 N2	05 BENZIDINE
PP	8	180	C6 H3 CL3	08 1,2,4-TRICHLOROBENZENE
PP	9	282	C6 CL6	09 HEXACHLOROBENZENE
PP	12	234	C2 CL6	12 HEXACHLOROETHANE
PP	18	142	C4 H8 O CL2	18 BIS(2-CHLOROETHYL)ETHER
PP	20	162	C10 H7 CL	20 2-CHLORONAPHTHALENE
PP	25	146	C6 H4 CL2	25 1,2-DICHLOROBENZENE
PP	26	146	C6 H4 CL2	26 1,3-DICHLOROBENZENE
PP	27	146	C6 H4 CL2	27 1,4-DICHLOROBENZENE
PP	28	252	C12 H10 N2 CL2	28 3,3'-DICHLOROBENZIDINE
PP	35	182	C7 H6 O4 N2	35 2,4-DINITROTOLUENE
PP	36	182	C7 H6 O4 N2	36 2,6-DINITROTOLUENE
PP	37	182	C12 H10 N2	37 1,2-DIPHENYLHYDRAZINE (MEAS AS AZOB
PP	39	202	C16 H10	39 FLUORANTHENE
PP	40	204	C12 H9 O CL	40 4-CHLOROPHENYL PHENYL ETHER
PP	41	248	C12 H9 O BR	41 4-BROMOPHENYL PHENYL ETHER
PP	42	170	C6 H12 O CL2	42 BIS(2-CHLOROISOPROPYL)ETHER
PP	43	172	C5 H10 O2 CL2	43 BIS(2-CHLOROETHOXY)METHANE
PP	52	258	C4 CL6	52 HEXACHLOROBUTADIENE
PP	53	270	C5 CL6	53 HEXACHLOROCYCLOPENTADIENE
PP	54	138	C9 H14 O	54 ISOPHORONE
PP	55	128	C10 H8	55 NAPHTHALENE
PP	56	123	C6 H5.O2 N	56 NITROBENZENE
PP	62	169	C12 H11.N	62 N-NITROSODIPHENYLAMINE (MEAS AS DIP
PP	63	130	C6 H14 O N2	63 N-NITROSODIPROPYLAMINE
PP	66	390	C24 H38 O4	66 BIS(2-ETHYLHEXYL)PHTHALATE
PP	67	312	C18 H20 O4	67 BUTYL BENZYL PHTHALATE
PP	68	278	C16 H22 O4	68 DI-N-BUTYLPHTHALATE
PP	69	390	C24 H38 O4	69 DI-N-OCTYLPHTHALATE
PP	70	222	C12 H14 O4	70 DIETHYLPHTHALATE
PP	71	194	C10 H10 O4	71 DIMETHYLPHTHALATE
PP	72	228	C18 H12	72 BENZO(A)ANTHRACENE
PP	73	252	C20 H12	73 BENZO\A\PYRENE
PP	74	252	C20 H12	74 3,4-BENZOFLUORANTHENE
PP	75	252	C20 H12	75 BENZO\K\FLUORANTHENE
PP	76	228	C18 H12	76 CHRYSENE
PP	77	152	C12 H8	77 ACENAPHTHYLENE
PP	78	178	C14 H10	78 ANTHRACENE
PP	80	166	C13 H10	80 FLUORENE
PP	81	178	C14 H10	81 PHENANTHRENE
PP	84	202	C16 H10	84 PYRENE
PP	130	188	C14 D10	SUB D10-PHENANTHRENE (130)
PP	136	136	C8 D8	ISB D8-NAPHTHALENE (136)

INPUT FILE: PPVOL.LL, OUTPUT FILE: PPVOL.LL

PP,	122	PP,	2	PP,	3	PP,	4	PP,	6	PP,	7
PP,	10	PP,	11	PP,	13	PP,	14	PP,	15	PP,	16
PP,	23	PP,	29	PP,	30	PP,	32	PP,	38	PP,	44
PP,	45	PP,	46	PP,	47	PP,	48	PP,	49	PP,	51
PP,	85	PP,	86	PP,	87	PP,	88	PP,	141	PP,	123

NAM	NUM:	WT	FORMULA	NAME
PP	122:	126	C4. H8. CL2	ISV 1,4-DICHLOROBUTANE (122)
PP	2:	56	C3. H4. O	02 ACROLEIN
PP	3:	53	C3. H3. N	03 ACRYLONITRILE
PP	4:	78	C6. H6	04 BENZENE
PP	6:	152	C. CL4	06 CARBONTETRACHLORIDE
PP	7:	112	C6. H5. CL	07 CHLOROBENZENE
PP	10:	98	C2. H4. CL2	10 1,2-DICHLOROETHANE
PP	11:	132	C2. H3. CL3	11 1,1,1-TRICHLOROETHANE
PP	13:	98	C2. H4. CL2	13 1,1-DICHLOROETHANE
PP	14:	132	C2. H3. CL3	14 1,1,2-TRICHLOROETHANE
PP	15:	166	C2. H2. CL4	15 1,1,2,2-TETRACHLOROETHANE
PP	16:	64	C2. H5. CL	16 CHLOROETHANE
PP	23:	118	C. H. CL3	23 CHLOROFORM
PP	29:	96	C2. H2. CL2	29 1,1-DICHLOROETHENE
PP	30:	96	C2. H2. CL2	30 1,2-TRANS-DICHLOROETHYLENE
PP	32:	112	C3. H6. CL2	32 1,2-DICHLOROPROPANE
PP	38:	106	C8. H10	38 ETHYLBENZENE
PP	44:	84	C. H2. CL2	44 METHYLENECHLORIDE
PP	45:	50	C. H3. CL	45 METHYL CHLORIDE
PP	46:	94	C. H3. BR	46 METHYL BROMIDE
PP	47:	250	C. H. BR3	47 BROMOFORM
PP	48:	162	C. H. CL2. BR	48 BROMODICHLOROMETHANE
PP	49:	136	C. CL3. F	49 TRICHLOROFLUOROMETHANE
PP	51:	206	C. H. CL. BR2	51 DIBROMOCHLOROMETHANE
PP	85:	164	C2. CL4	85 TETRACHLOROETHENE
PP	86:	92	C7. H8	86 TOLUENE
PP	87:	130	C2. H. CL3	87 TRICHLOROETHENE
PP	88:	62	C2. H3. CL	88 VINYLCHLORIDE
PP	141:	41	C2. H3. N	SPV ACETONITRILE (141)
PP	123:	128	C. H2. CL. BR	ISV BROMOCHLOROMETHANE (123)

INPUT FILE: PPPH.LL, OUTPUT FILE: PPPH.LL

PP,	133	PP,	135	PP,	21	PP,	22	PP,	24	PP,	31
PP,	34	PP,	57	PP,	58	PP,	59	PP,	60	PP,	64
PP,	65	PP,	134								

NAM	NUM:	WT	FORMULA	NAME
PP	133:	188	C14. D10	ISA D10-PHENANTHRENE (133)
PP	135:	136	C8. D8	ISA D8-NAPHTHALENE (135)
PP	21:	196	C6. H3. O. CL3	21 2,4,6-TRICHLOROPHENOL
PP	22:	142	C7. H7. O. CL	22 4-CHLORO-3-METHYLPHENOL
PP	24:	128	C6. H5. O. CL	24 2-CHLOROPHENOL
PP	31:	162	C6. H4. O. CL2	31 2,4-DICHLOROPHENOL
PP	34:	122	C8. H10. O	34 2,4-DIMETHYLPHENOL
PP	57:	139	C6. H5. O3. N	57 2-NITROPHENOL
PP	58:	139	C6. H5. O3. N	58 4-NITROPHENOL
PP	59:	184	C6. H4. O5. N2	59 2,4-DINITROPHENOL
PP	60:	198	C7. H6. O5. N2	60 4,6-DINITRO-O-CRESOL
PP	64:	264	C6. H. O. CL5	64 PENTACHLOROPHENOL
PP	65:	94	C6. H6. O	65A PHENOL
PP	134:	162	C7. H5. O. F3	SUA A,A,A-TRIFLUORO-M-CRESOL (134)

Volatiles in Water Library List

INPUT FILE: PPAIR.LL, OUTPUT FILE: PPAIR.LL

PP,	125	PP,	3	PP,	4	PP,	6	PP,	7	PP,	8
PP,	10	PP,	11	PP,	13	PP,	14	PP,	15	PP,	18
PP,	23	PP,	29	PP,	30	PP,	32	PP,	38	PP,	44
PP,	47	PP,	85	PP,	86	PP,	87	PP,	142	PP,	143
PP,	144	PP,	145	PP,	146	PP,	147				

NAM	NUM:	WT	FORMULA	NAME
PP	125:	186	C6. F6	AIS HEXAFLUOROBENZENE (125)
PP	3:	53	C3. H3. N	03 ACRYLONITRILE
PP	4:	78	C6. H6	04 BENZENE
PP	6:	152	C. CL4	06 CARBONTETRACHLORIDE
PP	7:	112	C6. H5. CL	07 CHLOROBENZENE
PP	8:	180	C6. H3. CL3	08 1,2,4-TRICHLOROBENZENE
PP	10:	98	C2. H4. CL2	10 1,2-DICHLOROETHANE
PP	11:	132	C2. H3. CL3	11 1,1,1-TRICHLOROETHANE
PP	13:	98	C2. H4. CL2	13 1,1-DICHLOROETHANE
PP	14:	132	C2. H3. CL3	14 1,1,2-TRICHLOROETHANE
PP	15:	166	C2. H2. CL4	15 1,1,2,2-TETRACHLOROETHANE
PP	18:	142	C4. H8. O. CL2	18 BIS(2-CHLOROETHYL)ETHER
PP	23:	118	C. H. CL3	23 CHLOROFORM
PP	29:	96	C2. H2. CL2	29 1,1-DICHLOROETHENE
PP	30:	96	C2. H2. CL2	30 1,2-TRANS-DICHLOROETHYLENE
PP	32:	112	C3. H6. CL2	32 1,2-DICHLOROPROPANE
PP	38:	106	C8. H10	38 ETHYLBENZENE
PP	44:	84	C. H2. CL2	44 METHYLENECHLORIDE
PP	47:	250	C. H. BR3	47 BROMOFORM
PP	85:	164	C2. CL4	85 TETRACHLOROETHENE
PP	86:	92	C7. H8	86 TOLUENE
PP	87:	130	C2. H. CL3	87 TRICHLOROETHENE
PP	142:	58	C3. H6. O	SPA ACETONE (142)
PP	143:	86	C6. H14	SPA HEXANE
PP	144:	128	C. H2. CL. BR	SPA BROMOCHLOROMETHANE (144)
PP	145:	246	C6. BR. F5	SPA BROMOPENTAFLUOROBENZENE (145)
PP	146:	126	C4. H8. CL2	SPA 1,4-DICHLOROBUTANE (146)
PP	147:	136	C. CL3. F	SPA FLUOROTRICHLOROMETHANE (147)

INPUT FILE: PP.LL, OUTPUT FILE PP.LL

PP,	1	PP,	2	PP,	3	PP,	4	PP,	5	PP,	6
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PP,	13	PP,	14	PP,	15	PP,	16	PP,	17	PP,	18
PP,	19	PP,	20	PP,	21	PP,	22	PP,	23	PP,	24
PP,	25	PP,	26	PP,	27	PP,	28	PP,	29	PP,	30
PP,	31	PP,	32	PP,	33	PP,	34	PP,	35	PP,	36
PP,	37	PP,	38	PP,	39	PP,	40	PP,	41	PP,	42
PP,	43	PP,	44	PP,	45	PP,	46	PP,	47	PP,	48
PP,	49	PP,	50	PP,	51	PP,	52	PP,	53	PP,	54
PP,	55	PP,	56	PP,	57	PP,	58	PP,	59	PP,	60
PP,	61	PP,	62	PP,	63	PP,	64	PP,	65	PP,	66
PP,	67	PP,	68	PP,	69	PP,	70	PP,	71	PP,	72
PP,	73	PP,	74	PP,	75	PP,	76	PP,	77	PP,	78
PP,	79	PP,	80	PP,	81	PP,	82	PP,	83	PP,	84
PP,	85	PP,	86	PP,	87	PP,	88	PP,	89	PP,	90
PP,	91	PP,	92	PP,	93	PP,	94	PP,	95	PP,	96
PP,	97	PP,	98	PP,	99	PP,	100	PP,	101	PP,	102
PP,	103	PP,	104	PP,	105	PP,	106	PP,	107	PP,	108
PP,	109	PP,	110	PP,	111	PP,	112	PP,	113	PP,	114
PP,	115	PP,	116	PP,	117	PP,	118	PP,	119	PP,	120
PP,	121	PP,	122	PP,	123	PP,	124	PP,	125	PP,	126
PP,	127	PP,	128	PP,	129	PP,	130	PP,	131	PP,	132
PP,	133	PP,	134	PP,	135	PP,	136	PP,	137	PP,	138
PP,	139	PP,	140	PP,	141	PP,	142	PP,	143	PP,	144
PP,	145	PP,	146	PP,	147						

NAM	NUM:	WT	FORMULA		NAME
PP	1:	154	C12.H10	01	ACENAPHTHENE
PP	2:	56	C3.H4.O	02	ACROLEIN
PP	3:	53	C3 H3.N	03	ACRYLONITRILE
PP	4:	78	C6.H6	04	BENZENE
PP	5:	184	C12.H12.N2	05	BENZIDINE
PP	6.	152	C.CL4	06	CARBONTETRACHLORIDE
PP	7:	112	C6.H5.CL	07	CHLOROBENZENE
PP	8:	180	C6.H3.CL3	08	1,2,4-TRICHLOROBENZENE
PP	9:	282	C6.CL6	09	HEXACHLOROBENZENE
PP	10:	98	C2.H4.CL2	10	1,2-DICHLOROETHANE
PP	11·	132	C2 H3.CL3	11	1,1,1-TRICHLOROETHANE
PP	12:	234	C2.CL6	12	HEXACHLOROETHANE
PP	13·	98	C2.H4.CL2	13	1,1-DICHLOROETHANE
PP	14·	132	C2.H3 CL3	14	1,1,2-TRICHLOROETHANE
PP	15:	166	C2.H2.CL4	15	1,1,2,2-TETRACHLOROETHANE
PP	16:	64	C2.H5.CL	16	CHLOROETHANE
PP	17:	114	C2.H4.O CL2	17	BIS(CHLOROMETHYL) ETHER
PP	18:	142	C4.H8.O.CL2	18	BIS(2-CHLOROETHYL)ETHER
PP	19·	106	C4.H7 O.CL	19	2-CHLOROETHYL VINYL ETHER
PP	20	162	C10.H7.CL	20	2-CHLORONAPHTHALENE
PP	21:	196	C6.H3.O.CL3	21	2,4,6-TRICHLOROPHENOL
PP	22:	142	C7.H7.O.CL	22	4-CHLORO-3-METHYLPHENOL
PP	23:	118	C.H.CL3	23	CHLOROFORM
PP	24:	128	C6.H5 O.CL	24	2-CHLOROPHENOL
PP	25:	146	C6.H4.CL2	25	1,2-DICHLOROBENZENE
PP	26:	146	C6.H4.CL2	26	1,3-DICHLOROBENZENE
PP	27:	146	C6 H4.CL2	27	1,4-DICHLOROBENZENE
PP	28:	252	C12.H10.N2.CL2	28	3,3'-DICHLOROBENZIDINE
PP	29:	96	C2.H2.CL2	29	1,1-DICHLOROETHENE
PP	30.	96	C2.H2.CL2	30	1,2-TRANS-DICHLOROETHYLENE
PP	31:	162	C6.H4.O.CL2	31	2,4-DICHLOROPHENOL
PP	32:	112	C3 H6.CL2	32	1,2-DICHLOROPROPANE
PP	33:	110	C3.H4.CL2	33	1,3-CIS-DICHLOROPROPENE
PP	34:	122	C8.H10.O	34	2,4-DIMETHYLPHENOL
PP	35:	182	C7.H6.O4.N2	35	2,4-DINITROTOLUENE
PP	36:	182	C7.H6.O4.N2	36	2,6-DINITROTOLUENE
PP	37:	182	C12.H10.N2	37	1,2-DIPHENYLHYDRAZINE (MEAS. AS AZOB
PP	38:	106	C8.H10	38	ETHYLBENZENE
PP	39:	202	C16.H10	39	FLUORANTHENE
PP	40.	204	C12.H9.O.CL	40	4-CHLOPOPHENYL PHENYL ETHER
PP	41:	248	C12.H9.O.BR	41	4-BROMOPHENYL PHENYL ETHER
PP	42:	170	C6 H12.O CL2	42	BIS(2-CHLOROISOPROPYL)ETHER
PP	43:	172	C5.H10.O2.CL2	43	BIS(2-CHLOROETHOXY)METHANE
PP	44.	84	C.H2 CL2	44	METHYLENECHLORIDE
PP	45.	50	C.H3.CL	45	METHYL CHLORIDE
PP	46·	94	C.H3.BR	46	METHYL BROMIDE
PP	47.	250	C H.BR3	47	BROMOFORM
PP	48:	162	C.H.CL2.BR	48	BROMODICHLOROMETHANE
PP	49:	136	C.CL3.F	49	TRICHLOROFLUOROMETHANE
PP	50	120	C CL2.F2	50	DICHLORODIFLUOROMETHANE
PP	51:	206	C H.CL.BR2	51	DIBROMOCHLOROMETHANE
PP	52:	258	C4.CL6	52	HEXACHLOROBUTADIENE
PP	53.	270	C5.CL6	53	HEXACHLOROCYCLOPENTADIENE
PP	54·	138	C9.H14.O	54	ISOPHORONE
PP	55·	128	C10.H8	55	NAPHTHALENE
PP	56:	123	C6.H5.O2.N	56	NITROBENZENE
PP	57·	139	C6.H5.O3.N	57	2-NITROPHENOL
PP	58:	139	C6.H5.O3.N	58	4-NITROPHENOL
PP	59:	184	C6.H4.O5 N2	59	2,4-DINITROPHENOL
PP	60·	198	C7.H6.O5.N2	60	4,6-DINITRO-O-CRESOL
PP	61:	74	C2.H6.O N2	61	N-NITPOSODIMETHYLAMINE
PP	62.	169	C12.H11 N	62	N-NITROSODIPHENYLAMINE (MEAS. AS DIP
PP	63.	130	C6.H14.O.N2	63	N-NITROSODIPROPYLAMINE
PP	64:	266	C6.H O CL5	64	PENTACHLORGPHENOL
PP	65:	94	C6.H6 O	65A	PHENOL
PP	66.	390	C24.H38.O4	66	BIS(2-ETHYLHEXYL)PHTHALATE
PP	67:	312	C18.H20.O4	67	BUTYL BENZYL PHTHALATE
PP	68:	278	C16 H22 O4	68	DI-N-BUTYLPHTHALATE

```
PP   69:  390 C24.H38.O4        69  DI-N-OCTYLPHTHALATE
PP   70:  222 C12.H14.O4        70  DIETHYLPHTHALATE
PP   71:  194 C10.H10.O4        71  DIMETHYLPHTHALATE
PP   72:  228 C18.H12           72  BENZO(A)ANTHRACENE
PP   73:  252 C20.H12           73  BENZO\A\PYRENE
PP   74:  252 C20.H12           74  3,4-BENZOFLUORANTHENE
PP   75.  252 C20.H12           75  BENZO\K\FLUORANTHENE
PP   76:  228 C18.H12           76  CHRYSENE
PP   77:  152 C12.H8            77  ACENAPHTHYLENE
PP   78:  178 C14.H10           78  ANTHRACENE
PP   79:  276 C22.H12           79  BENZO\GHI\PERYLENE
PP   80:  166 C13.H10           80  FLUORENE
PP   81:  178 C14.H10           81  PHENANTHRENE
PP   82:  278 C22.H14           82  DIBENZO\AH\ANTHRACENE
PP   83:  276 C22.H12           83  INDENO\1,2,3-CD\PYRENE
PP   84:  202 C16.H10           84  PYRENE
PP   85:  164 C2.CL4            85  TETRACHLOROETHENE
PP   86:   92 C7.H8             86  TOLUENE
PP   87:  130 C2.H.CL3          87  TRICHLOROETHENE
PP   88:   62 C2.H3.CL          88  VINYLCHLORIDE
PP   89:  362 C12.H8.CL6        89  ALDRIN
PP   90:  378 C12.H8.O.CL6      90  DIELDRIN
PP   91:  406 C10.H6.CL8        91  CHLORDANE
PP   92:  352 C14.H9.CL5        92  4,4'-DDT
PP   93:  316 C14.H8.CL4        93  4,4'-DDE
PP   94:  318 C14.H10.CL4       94  4,4'-DDD
PP   95:  404 C9.H6.O3.S.CL6    95  A-ENDOSULFAN-ALPHA
PP   96:  404 C9.H6.O3.S.CL6    96  B-ENDOSULFAN-BETA
PP   97:    0                   DUMMY ENTRY
PP   98:  378 C12.H8.O.CL6      98  ENDRIN
PP   99:  392 C12.H5.O2.CL6     99  ENDRIN ALDEHYDE
PP  100:  370 C10.H5.CL7        100 HEPTACHLOR
PP  101:    0                   DUMMY ENTRY
PP  102:  288 C6.H6.CL6         102 A-BHC-ALPHA
PP  103:    0                   DUMMY ENTRY
PP  104:  288 C6.H6.CL6         104 G-BHC-GAMMA
PP  105:    0                   DUMMY ENTRY
PP  106:  256 C12.H7.CL3        106 PCB-1242
PP  107:  324 C12.H5.CL5        107 PCB-1254
PP  108:  183 C12.H9.CL         108 PCB-1221
PP  109:  188 C12.H7.CL         109 PCB-1232
PP  110:  290 C12.H6.CL4        110 PCB-1248
PP  111:  392 C12.H3.CL7        111 PCB-1260
PP  112:  256 C12.H7.CL3        112 PCB-1016
PP  113:  320 C12.H4.O2.CL4     129 2,3,7,8,-TETRACHLORODIBENZO-P-DIOXIN
PP  114:  110 C3.H4.CL2         33A 1,3-TRANS-DICHLOROPROPENE
PP  115:    0                   DUMMY ENTRY
PP  116:    0                   DUMMY ENTRY
PP  117:    0                   DUMMY ENTRY
PP  118:    0                   DUMMY ENTRY
PP  119:    0                   DUMMY ENTRY
PP  120:    0                   DUMMY ENTRY
PP  121:  188 C14.D10               D10-ANTHRACENE (INTERNAL STANDARD) 1
PP  122:  126 C4.H8.CL2         ISV 1,4-DICHLOROBUTANE (122)
PP  123:  128 C.H2.CL.BR        ISV BROMOCHLOROMETHANE (123)
PP  124:  188 C14.D10           ISA D10-ANTHRACENE (124)
PP  125:    0                   AIS HEXAFLUOROBENZENE  (125)
PP  126:    0                   DUMMY ENTRY
PP  127:    0                   DUMMY ENTRY
PP  128:    0                   DUMMY ENTRY
PP  129:    0                   DUMMY ENTRY
PP  130:  188 C14.D10               D10-PHENANTHRENE (INTERNAL STANDARD)
PP  131:  150 C6 CL2.D4             D4-1,4-DICHLOROBENZENE (INTERNAL STA
PP  132:  164 C12.D10               D10-BIPHENYL (INTERNAL STANDARD) 132
PP  133:    0                   DUMMY ENTRY
PP  134:    0                   DUMMY ENTRY
PP  135:    0                   DUMMY ENTRY
PP  136:    0                   DUMMY ENTRY
PP  137:    0                   DUMMY ENTRY
PP  138:    0                   DUMMY ENTRY
```

```
PP  139:    0                       DUMMY ENTRY
PP  140:    0                       DUMMY ENTRY
PP  141:   41 C2.H3.N               SPV ACETONITRILE  (141)
PP  142:   58 C3.H6.O               SPA ACETONE  (142)
PP  143:   86 C6.H14                SPA HEXANE  (143)
PP  144:  128 C.H2.CL.BR            SPA BROMOCHLOROMETHANE (144)
PP  145:  246 C6.BR.F5              SPA BROMOPENTAFLUOROBENZENE (145)
PP  146:  126 C4.H8.CL2             SPA 1,4-DICHLOROBUTANE (146)
PP  147:  136 C.CL3.F               SPA FLUOROTRICHLOROMETHANE (147)
```

APPENDIX B

Operations of Procedure EVALØ

Procedure EVALØ

Typical Output of EVALØ

> EVALØ LIBRARY LIST, YES or NO (NB Library Search), YES or NO (Print Target Compound Spectra) is the command that executes the procedure.

EVALØ is the master evaluation procedure that processes data files that are stored in name list EVAL.

```
> EDNL Ø: EVAL  (CR)1/
EDNL:  N; FILENAME
EDNL: W;E
     or
> SETN Ø: EVAL
> FILE
FILE: D Ø: FILENAME
FILE: >
(Append file displayed to name list EVAL stored on Unit # Ø.)
```

This procedure processes a file by locating an internal standard (IS) within a fixed retention time window and by locating preselected or target compounds within fixed relative retention time windows. One internal standard is used for quantification of the target compounds. Relative retention times (RRT) for the target compounds are calculated relative to the internal standard used for quantitation. The internal standard(s) and target compounds are stored in a user library. The user library stores the compound name, its library entry number, molecular weight, formula, retention time, relative retention time, internal standard used for quantitation, compound ion used for quantitation, and response factor.

EVALØ is driven by a library list. A library list is a subset of the master user library containing the library entry numbers of compounds to be searched for by EVALØ. The target compounds in the library list are located in the data file and identified using relative retention time data and a reverse-search library procedure. In reverse-search the mass spectrum of a compound of interest is selected from a user created library and compared to mass spectra in the GC/MS run within a set relative retention time window. If the compound is located in the GC/MS run, the area of a preselected ion is measured and stored in a quantitation list. The procedure prints a copy of the reconstructed ion chromatogram (RIC), the mass spectrum of each target compound detected, the mass chromatogram of each target compound detected, and the quantitation and identification report for each file processed.

Compounds other than target compounds (unknowns) present in the sample can be compared to the entries in the National Bureau of Standards (NBS) library of mass spectra. If the analyst elects to identify unknown compounds in the sample, the procedure prints a comparison of unknown spectra to library spectra and a qualitative report listing the procedure's best identification of the compounds.

1/ (CR) - Carriage return. Each command to the system must be terminated with a carriage return.

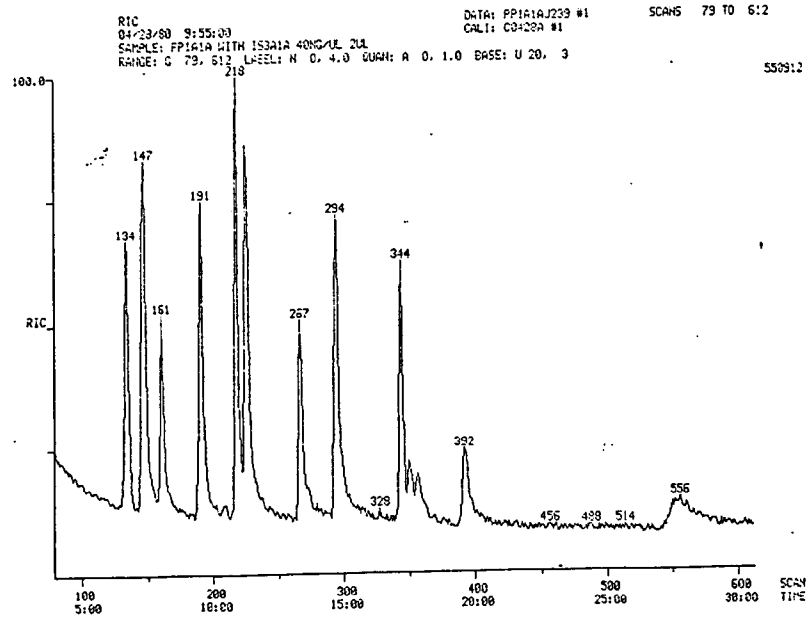
> EVALØ LIBRARY LIST, NO, NO gives the analyst the option of not printing target compound spectra at the time of initial processing. In this mode the procedure prints an RIC, the mass chromatogram of each preselected compound, and the quantitation and identification report for each file processed. The spectra can then be printed in batch overnight using procedure ESPEC. The above command also gives the analyst the option of not performing the NBS library search to identify unknown compounds. The qualitative report listing the best identification of unknown compounds can be generated by batch processing overnight using procedure ESPEC.

Create User Library

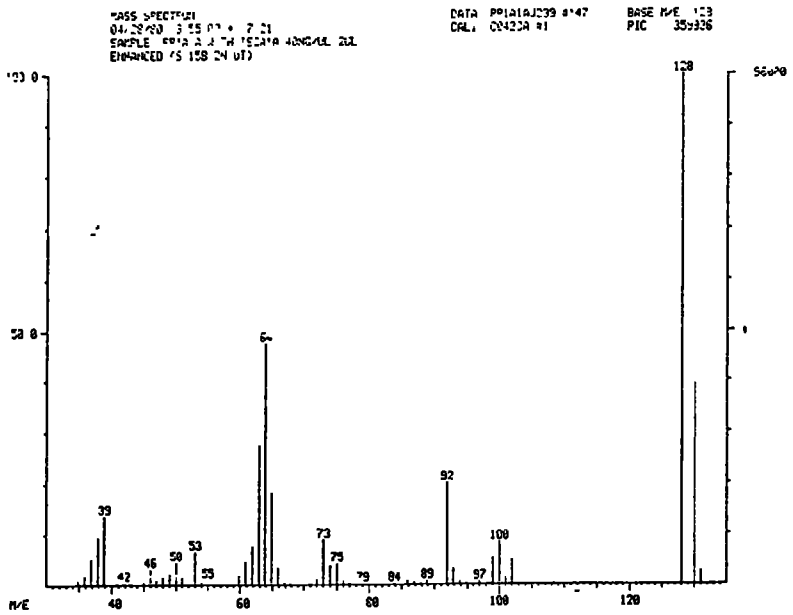
Label chromatogram with instrument name and type, GC/MS conditions, and injection volume.

Locate and identify all of the compounds using CHRO, SPEC, LIBR. Record the scan number of the internal standard used for quantification.

> CHRO PPIAIAJ239, CØ428A
(> CHRO data file, calibration file)



CHRO: S'147
(Get enhanced spectrum of scan #147)

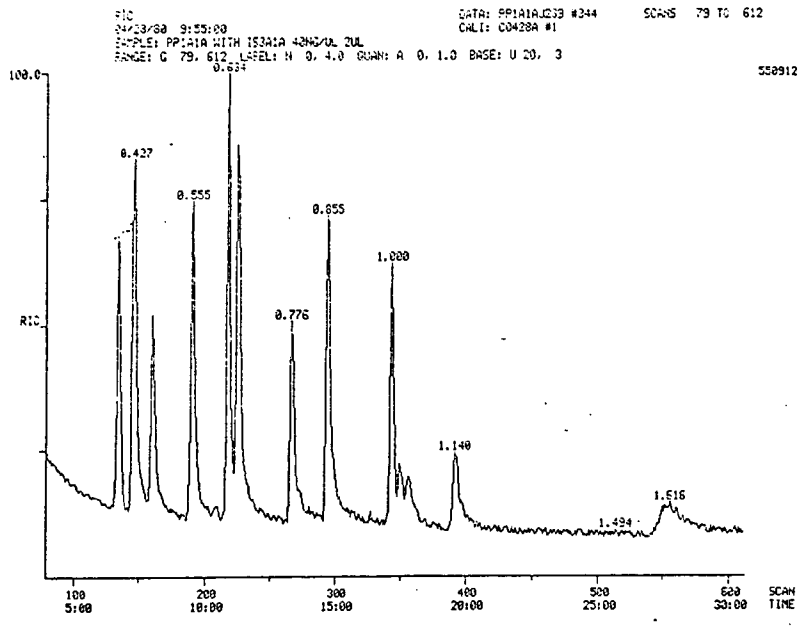


SPEC: Y
(Do forward library search on scan #147; search will list 3 compound matches according to best PURITY values.)

```
LIBRARY SEARCH                DATA  PP1A1AJ239 # 147     BASE M/E   128
04/28/80  9 55 00 +  7 21     CALI  C0428A #   1         RIC      345087
SAMPLE  PP1A1A WITH IS3A1A 40NG/UL 2UL
ENHANCED (S 15B 2N 0T)

25409 SPECTRA IN LIBRARYNB SEARCHED FOR MAXIMUM PURITY
  182 MATCHED AT LEAST 4 OF THE 16 LARGEST PEAKS IN THE UNKNOWN

RANK IN NAME
1   723 PHENOL, 2-CHLORO-
2  1169 PHENOL, 3-CHLORO-
3  1079 PHENOL, 4-CHLORO-
4  3357 BENZENE, 1-CHLORO-2-ETHOXY-
5  4277 ACETICACID, 4-CHLOROPHENYLESTER

RANK  FORMULA          M WT  B PK   PURITY   FIT   RFIT
1 C6 H5 O CL            128   128      878   935    914
2 C6 H5 O CL            128   128      852   923    879
3 C6 H5 O CL            128   128      831   911    860
4 C8 H9 O CL            156   123      645   729    871
5 C8 H7 O2 CL           170   128      567   682    775
```

When all of the compounds have been identified, calculate the RRT of each compound.

CHRO: X344; F2
(CHRO: Xscan number of IS; flag set to calculate RRT)



List all compounds in order of increasing priority pollutant number.

PP#	Compound	Scan	RT	RRT	Quantitation Mass	Standard Amt	Reference Peak
21	2,4,6-Trichlor-ophenol	267	13:21	0.778	196	100 ng/uL	-
22	4-Chloro-3-methylphenol	294	14:42	0.857	142	100 ng/uL	-
24	2-Chlorophenol	147	7:21	0.429	128	100 ng/uL	-

Create master user library containing the mass spectra of Priority Pollutants. At this point enter a temporary name for the library. Compounds will be entered into the library in order of elution. The entries will be rearranged in order of increasing priority pollutant number and the library given a permanent name after all the spectra have been entered.

```
> CHRO PPIAIAJ239, CØ428A
CHRO: S' 147
SPEC: Y
LIBR: ED
(Call library editor)
EDLB: #ZZ
(Set output library)
(Insert the current spectrum into the output library assigning it the first
number not already assigned.  A list of questions are presented.)


New Name: 24  2-Chlorophenol
(priority pollutant number   compound name)
New Formula:
Molecular Weight:
Relative Ret. Time:  0.429
Quantitation Mass:  128
Standard Amount:  100
Units:  ng/ul
```

Retention time and base peak intensity are input by the system. Reference peak and response factor are defaulted at this time.

```
EDLB: E
LIBR: E
CHRO: S' 161
(Examine next spectra; begin the process to enter this compound in the library.)
```

After all of the compounds have been entered into the library, check each entry.

```
EDLB: $ZZ; #ZZ
(Input Library, Output Library)
EDLB: G1
(Get the first entry in the Input Library.)  Check each entry in the library
for correctness of information.
```

If all the information in an entry is not correct, correct that entry and reinsert that entry into the library.

```
EDLB: I' 1

"Do you really want to overwrite entry 1 in Library ZZ?"
(Type Y is yes)
Y
```

The list of parameters will be presented for correction. The system will type:

```
"Overwriting entry #1 in Library ZZ, everything OK?"
(Type N if not)
EDLB: G2, G3, G4, etc.
(Inspect entries 2,3,4, etc. one at a time in the same manner as entry 1.)
```

ONCE AN ENTRY IS MADE IN A LIBRARY, IT CANNOT BE DELETED. IT CAN ONLY BE OVERWRITTEN.

After all of the standard reference compounds have been chromatographed and entered in the temporary user library ZZ, rearrange the master user library in order of increasing priority pollutant number. Reserve entries 115 through 140 for internal standard entries. The spaces can be reserved by loading dummy entries having a single mass at 100 with an intensity of 1000 into those positions.

```
> EDLL PP
(Create new library list PP)
EDLL: $ZZ, 23
(Append library ZZ entry #23 to library list PP; this entry will become entry
#1 in the permanent library.)
EDLL: $ZZ, 30
(This entry will become entry #2 in the permanent library.)
```

Append all library entry numbers to the library list.

```
EDLL: D
(Display entries numbers in library list.)
EDLL: W
(Write current list to output file.)
EDLL: #PP
(Create master library named PP using current library list.)
EDLL: -
(Delete all entries in list.)
EDLL: $PP, 1, 140
(Append entries 1 through 140 to library list from Library PP.)
EDLL: D
(Examine entry numbers.)
```

If the numbers are correct:

```
EDLL: B
(Print list of entry number, molecular weight, formula, first 40 characters
of name.)
EDLL: W, E
(Write list to output file; exit.)
```

Create Library Lists

Create a library list for each standard reference mixture. The internal standard used for quantitation must be the first entry. Other internal standards may precede or follow the remaining standard reference compounds on the list. The standard reference compounds must be in order of increasing priority pollutant number.

> EDLL PPPH
(Create library list PPPH for priority pollutant acid fraction standard mixture.)
EDLL: $PP, 133
(Append entry #133 from Library PP to list.)
EDLL: $PP, 135
(Append entry #135 from Library PP to list.)

Append other compound names from standard mixture to the list.

Inspect the library entries referenced in the library list:

>EDLB PP
EDLB: G133
(Call entry #133 in Library PP.)

```
LIBRARY EDITOR                DATA  LIBRARYPP   133          BASE M/E   188
C14 D10                       M WT   188
NAME     ISA D10-PHENANTHRENE (133)
RET T        17 09  DP 1     29888    U P 1       --     U P 2       --
R R T     1 0000    MASS   188 0000   AMNT     40 0000   NG/UL
REF PK PP  133     R FAC     1 0000   INPUT  LIBRARYPP  OUTPUT LIBRARYPP

MASS INTENSITY  MASS INTENSITY   MASS INTENSITY  MASS INTENSITY
  52     32        94   164        136    19        183    36
  64     24       100    24        146    29        184   160
  66     60       102    21        156   107        186   137
  76     37       106    17        158   145        188  1000
  78     62       108    15        160   160        189   129
  80    167       118    13        161    30
  90     39       130    17        180    24
  92     99       132    39        182    34
```

Check retention time, relative retention time, quantitation mass, and standard amount. A value for the reference peak should be entered at this time.

REF PEAK (NAME, NUM): PP, 133
(Entry #133 in Library PP is the internal standard used in quantitating this standard reference mixture.)

Execute EVALØQ

The command needed to execute EVALØQ is > EVALØQ FILENAME, LIBRARY LIST

EVALØQ.PR is a prescreening procedure for EVALØ.PR. The procedure produces a QUAN list and a quantitation report for the standard mixture.

Inspect the QUAN list.

INPUT FILE PP1A1AJ239 QL, OUTPUT FILE PP1A1AJ239 QL

REFERENCE RETENTION TIME (MIN SEC) 6 42

NO	LOW MASS	HIGH	SCAN	TIME	METH	AREA	HEIGHT	NAME	NUM
1	187 56	188 56	343	17 09	A BB	336606	91008	PP	133
2	135 54	136 54	134	6 42	A BB	486994	146688	PP	135
3	195 56	196 56	267	13 21	A BB	66258	19020	PP	21
4	141 54	142 54	294	14 42	A BB	211184	57856	PP	22
5	127 54	128 54	147	7 21	A BB	374173	100962	PP	24
6	161 55	162 55	225	11 15	A BB	220935	65705	PP	31
7	121 54	122 54	218	10 54	A BB	271617	82291	PP	34
8	138 54	139 54	161	8 03	A BB	115756	37568	PP	57
9	265 50	266 50	392	19 36	A BB	21734	4040	PP	64
10	93 53	94 53	191	9 33	A BB	449189	121666	PP	65
11	138 54	139 54	554	27 42	A BB	21707	2030	PP	58
12	197 56	198 56	356	17 48	A VB	15153	2815	PP	60

Check the list to be sure that all of the standard compounds are present. Delete duplicates and extraneous peaks. If a compound is not listed as found, determine the reason. If a standard compound has not been detected, delete that compound entry from the QUAN list. If the standard compound can be identified and quantitated manually, append the compound name and quantitation results to the QUAN list using the procedure MQSA.PR.

> MQSA FILENAME#SCAN, LIBRARY NAME, #LIBRARY ENTRY is the command needed.

After the QUAN list has been edited, update response factors and relative retention times, and retention times.

> QUAN PPIAIAJ239
QUAN: R(1, 12)
(Update response factors for entries 1-12)
QUAN: S(1, 12)
(Update relative retention times for entries 1-12)
QUAN: T(1, 12)
(Update retention time for entries 1-12)

Execute EVALØ

> EVALØ LIBRARY LIST, YES or NO (NBS search), YES or NO (Print Spectra) is the command that executes the procedure.

EVALØ.PR is the master evaluation procedure. This procedure prints a copy of the reconstructed ion chromatogram, the mass spectrum of each target compound listed in the standard reference mixture library list, and a quantitation and identification report for each file processed.

Load the standard data filename into name list EVAL. The name list stores data files to be processed. Execute procedure EVALØ.

Inspect the QUAN list generated. Determine if all the standard compounds are present. If a compound is not listed as found, locate the peak manually and add the compound name and quantitation results to the QUAN list using the procedure MQSA.PR. Delete extraneous and duplicate entries from the QUAN list.

After the QUAN list has been edited, use the data system to update response factors, relative retention times, and retention times.

WARNING: DO NOT UPDATE "NOT FOUND" OR Ø ENTRIES.

```
> QUAN PPIAIAJ239
QUAN:  I; F2; H
```

```
QUANTITATION REPORT          FILE  PP1A1AJ239

DATA  PP1A1AJ239 TI
04/28/80  9 55 00
SAMPLE  PP1A1A WITH IS3A1A 40NG/UL 2UL
CONDS   70-190 8C/MIN
FORMULA                      INSTRUMENT  3200EI          WEIGHT     0 000
SUBMITTED BY  JFC            ANALYST  JFC               ACCT  NO   J239

AMOUNT=AREA * REF AMNT/(REF AREA* RESP FACT)

 NO  NAME
  1  ISA D10-PHENANTHRENE (133)
  2  ISA D8-NAPHTHALENE (135)
  3  21  2,4,6-TRICHLOROPHENOL
  4  22  4-CHLORO-3-METHYLPHENOL
  5  24  2-CHLOROPHENOL
  6  31  2,4-DICHLOROPHENOL
  7  34  2,4-DIMETHYLPHENOL
  8  57  2-NITROPHENOL
  9  64  PENTACHLOROPHENOL
 10  65A PHENOL
 11  58  4-NITROPHENOL
 12  60  4,6-DINITRO-O-CRESOL

 NO  M/E  SCAN   TIME  REF   RRT  METH      AREA      AMOUNT          %TOT
  1  188   343  17 09   1  1 000  A BB     336606   40 000 NG/UL     2 70
  2  136   134   6 42   1  0 391  A BB     486994   40 000 NG/UL     2 70
  3  196   267  13 21   1  0 778  A BB      66258  100 000 NG/UL     6 76
  4  142   294  14 42   1  0 857  A BB     211184  100 000 NG/UL     6 76
  5  128   147   7 21   1  0 429  A BB     374173  100 000 NG/UL     6 76
  6  162   225  11 15   1  0 656  A BB     220935  100 000 NG/UL     6 76
  7  122   218  10 54   1  0 636  A BB     271617  100 000 NG/UL     6 76
  8  139   161   8 03   1  0 469  A BB     115756  100 000 NG/UL     6 76
  9  266   392  19 36   1  1 143  A BB      21734  200 000 NG/UL    13 51
 10   94   191   9 33   1  0 557  A BB     449189  100 000 NG/UL     6 76
 11  139   554  27 42   1  1 615  A BB      21707  400 000 NG/UL    27 03
 12  198   356  17 48   1  1 038  A VB      15153  100 000 NG/UL     6 76

 NO  RET(L) RATIO RRT(L) RATIO    AMNT   AMNT(L)   R FAC R FAC(L) RATIO
  1  17 09  1 00  1 000  1 00   40 00    40 00   1 000   1 000   1 00
  2   6 42  1 00  0 391  1 00   40 00    40 00   1 447   1 447   1 00
  3  13 21  1 00  0 778  1 00  100 00   100 00   0 079   0 079   1 00
  4  14 42  1 00  0 857  1 00  100 00   100 00   0 231   0 251   1 00
  5   7 21  1 00  0 429  1 00  100 00   100 00   0 445   0 445   1 00
  6  11 15  1 00  0 656  1 00  100 00   100 00   0 263   0 263   1.00
  7  10 54  1 00  0 636  1 00  100 00   100 00   0 323   0 323   1 00
  8   8 03  1 00  0 469  1 00  100 00   100 00   0 138   0 138   1 00
  9  19 36  1 00  1 143  1 00  200 00   200 00   0 013   0 013   1 00
 10   9 33  1 00  0 557  1 00  100 00   100 00   0 534   0 534   1 00
 11  27 42  1 00  1 615  1 00  400 00   400 00   0 006   0 006   1 00
 12  17 48  1 00  1 038  1 00  100 00   100 00   0 018   0 018   1 00
```

After the data system has been standardized using the standard reference mix, samples and quality control samples can be evaluated. Load the data files to be processed into name list EVAL. Execute procedure EVALØ.

```
TRACE OF PROCEDURE EVALØ
   * ERASE
   * ,[PROCEDURE EVALØ                                                          ]
   * ,[WRITTEN 9/4/79 BY O J LOGSDON II, LAST REVISION 04/17/8Ø BAH             ]
   * ,[US EPA/NATIONAL ENFORCEMENT INVESTIGATIONS CENTER 303-234-4661           ]
   * ,[                                                                        ]
   * ;[   TO PROCESS DATA ON DISC DRIVE UNIT Ø, USE THIS PROCEDURE             ]
   * ,[  >EVALØ LIBRARYLIST,YES OR NO (NB SEARCH) YES OR NO (PRINT SPECTRA)    ]
   * ,[   WHERE THE LIBRARYLIST CONTAINS AT A MINIMUM AN INTERNAL STANDARD.    ]
   * ,[         OTHER PEAKS SUCH AS PRIORITY POLLUTANTS MAY BE INCLUDED FOR    ]
   * ;[         QUANTITATION AND IDENTIFICATION   NB SEARCH OF ANY LABELED BUT]
   * ;[         UNIDENTIFIED PEAKS DURING THE QUANTITATION MAY BE SELECTED     ]
   * ,[         ALSO, PRINTOUT OF THE IDENTIFIED SPECTRA FROM THE QUANTITATION]
   * ;[         RUN MAY BE SUPRESSED WITH A 'NO' RESPONSE ('YES' REQUIRED      ]
   * ,[         OTHERWISE)                                                     ]
   * ,SETQ TEMP
   * ;EDNL EVTEMP (-,$3,$2,$1,W,E)
   * ,EDSL TEMP(-,W,E)
   * ,EDSL YES (-,1,W,E),
   *  EDSL NO (-,W,E)
   * ,SET11 #Ø
   * ;SET12 #Ø
   * ,EVALØA
   * ;FEED,BEEP,BEEP,BEEP
   * ;ERASE,[PROCEDURE EVALO IS DONE]
   *
   ERASE
   SETQ TEMP
   EDNL EVTEMP (-,$3,$2,$1,W,E)
   EDSL TEMP (-;W,E)
   EDSL YES (-;1,W,E)
   EDSL NO (-;W,E)
   SET11
   SET12
   EVALØA
      * ;[ PART OF EVALØ \MAIN PROCESSING LOOP\ ]
      * ,SETN EVAL,SET5 '11,GETN,SET11 '5
      * ;EDLL $1(-,W,E)
      * ;EVALØB
      * ,LOOP
      *
      SETN EVAL
      SET5 '11
      GETN
      SET11 !5
      EDLL $1 (-,W;E)
      EVALØB
         * ,[ PART OF EVALØ \SETUP AND PROCESSING\ ]
         * ;PARA(I,H,E)
         * ,CHRO(H1,2ØØØ,E)
         * ,SETS $1,EDSL(-,W,E)
         * ,FILE(K PRIN 99/N,E),EDGL $1 (-,W,E)
         * ,MAP(I,F1;U1ØØØ,V2ØØØØØ,35,3ØØ,N>2,3,5,H1,2ØØØ,500,E)
         * ,SET3 $1,SETN EVTEMP,GETN #3,SETL $1#0,GETN #1,SETS $1,SET1 $3
         * ,EVALØC
         * ,EVALØD
         * ,EDLL (B'1,E)
         * ,PRIN(@P1),FILE(C PRIN 99,M /N,E),FEED
         * ,GUAN $1(I,F2,H,E)
         * ,EVALMØ
         * ,SET3 $1,SETN EVTEMP,GETN #2,SETS $1,SET1 $3
         * ,EVALØE
```

```
* ,EDSL $1(-,'12,A,E)
* ,EDSL TEMP,$1(A,E)
* ,EDSL TEMP(-,W,E)
* ,BEEP
*
PARA  (I,H,E)
CHRO  (H1,2000,E)
SETS $1
EDSL  (-,W,E)
FILE  (K PRIN 99/N,E)
EDQL $1 (-,W,E)
MAP   (I,F1,U1000,V200000,35,300,N>2,3,5,H1,2000,500,E)
SET3 $1
SETN EVTEMP
GETN #3
SETL $1
GETN #1
SETS $1
SET1 $3
EVALOC
   * ,[ PART OF EVALØ \LOCATE INTERNAL STD\ ]
   * ,SET14 #0
   * ,GETL
   * ,SEAR/V(I,$,&,V4000000,N2,10,500,D-25,25,E)
   * ,EVALOF
   * ,SET10 '14,SETL #0
   *
   SET14
   GETL
   SEAR  (I,$,&,V4000000,N2,10,500,D-25,25,E)/V
   EVALOF
      * ,[ PART OF EVALØ \ ?? INT  STD FOUND ?? \ ]
      * ,IF EVALOF #1,'14
      * ,PRIN(@P2),BEEP,BEEP;BEEP,BEEP
      * ,RETU EVALOB
      *
      IF EVALØF#1,'14
      PRIN  (@P2)
      BEEP
      BEEP
      BEEP
      BEEP
      RETU EVALØB
   SET10 '14
   SETL
EVALØD
   * ,[ PART OF EVALØ \DETECT SELECTED COMPOUNDS \ ]
   * ,SET1 '10,SET14 #0
   * ,GETL
   * ,SEAR/V(I,$,%,V4000000,N1,10,10,D-10,10,E)
   * ,PRIN/KX('4,2,'14,6,'15,6,'16,6,C,E)
   * ,EVALØG
   * ,LOOP
   *
   SET1 '10
   SET14
   GETL
   SEAR  (I,$,%,V4000000,N1,10,10,D-10,10,E)/V
   PRIN  ('4,2,'14,6,'15,6,'16,6,C,E)/KX
   EVALØG
      * ,[ PART OF EVALØ \QUANT LOOP ENTRY\ ]
      * ,EVALOH,EDQL $1(-,N,#,A,E)
      *
      EVALØH
         * ,[ PART OF EVALØ \MATCH CHECK AND QUANT\ ]
         * ,[CHANGE THE NUMBER '#800' TO DESIRED LEVEL OF COMPUTER MATCH]
```

```
            * ,IF EVALOH '16,EVALOH #80Ø
            * ,SET1 '14
            * ,EDSL TEMP(-,'14,A,E)
            * ,EDLL $1(-,$,A,E)
            * ,EDGL(-,W,E)
            * ,CHRO(I,R,$,#,N1,2,A>5,3,G-4,4,D-1Ø,1Ø,E)
            * ,EVALØI,RETU EVALOG
            *
            IF EVALOH'16,EVALØH#6ØØ
            SET1 '14
            EDSL TEMP (-,'14,A,E)
            EDLL $1 (-,$;A,E)
            EDGL  (-,W,E)
            CHRO  (I,R,$,#,N1,2,A>5,3,G-4,4,D-1Ø,1Ø,E)
            EVALOI
               * ,[ PART OF EVALO \SPECTRUM PRINTOUT\ ]
               * ,IF EVALØH '28,EVALOH
               * ,EDGL TEMP,$1(U+20,1ØØ,A,E)
               * ,EDSL $1(I,-'1,4,W,E)
               * ,IF EVALOI '27,EVALØI
               * ,LIBR(',I,N-,C,DS,HS,E)
               *
               IF EVALØH'28,EVALØH
               EDGL TEMP,$1 (U+20,1ØØ,A,E)
               EDSL $1 (I,-'1,4,W,E)
               IF EVALØI'27,EVALOI
               LIBR  (',I,N-,C,DS,HS,E)
            RETU EVALOG
         EDGL $1 (-,N,#,A,E)
      LOOP
EDLL  (B'1,E)
PRIN  (@P1)
FILE  (C PRIN 99,M /N,E)
FEED
QUAN $1 (I,F2,H,E)
EVALMO
      * SETL #Ø,SET1Ø #Ø
      * ,EVALM1
      * ,CHRO(H,I,E)
      *
      SETL
      SET1Ø
      EVALM1
         * GETL
         * ,CHRO($,K,E)
         * ,EVALM2
         * ,LOOP
         *
         GETL
         CHRO  ($,K,E)
         EVALM2
            * SET1Ø '1Ø#1
            * ;IF '10 EVALM2,#10
            * ,CHRO(H,I,E)
            * ;SET10 #Ø
            *
            SET1Ø #1'1Ø
            IF EVALM2'10,#1Ø
            CHRO  (H,I,E)
            SET10
         LOOP
      CHRO  (H,I,E)
SET3 $1
SETN EVTEMP
GETN #2
SETS $1
```

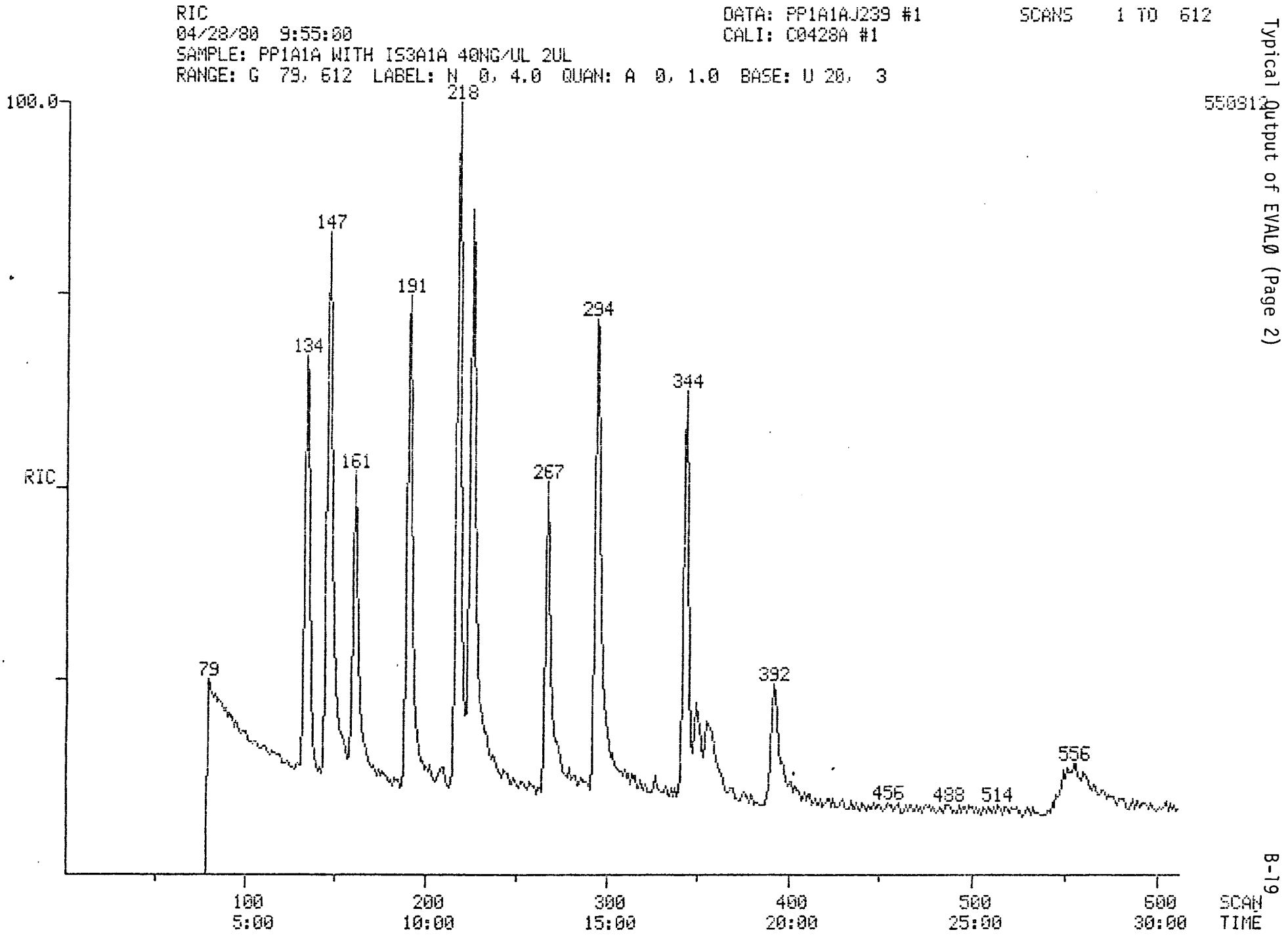
```
      SET1 $3
      EVALOE
         * ,[ PART OF EVALO \SELECT 'NB' SEARCH?\ ]
         * ,IF EVALOE '27,EVALOE
         * ,SET4 NB,SETL TEMP,EDQL $1,EVAL(I,-2,1000,W,E),SETS $1
         * ,EVALOJ
         * ,QUAN EVAL (I,H,E)
         *
         IF EVALOE'27,EVALOE
         SET4 NB
         SETL TEMP
         EDQL $1,EVAL (I,-2,1000,W,E)
         SETS $1
         EVALOJ
            * ,[ PART OF EVALO \'NB' SEARCH LOOP\ ]
            * ,GETS
            * ,LIBR(I,',F,N-,X2,3,H,HS,J<1,E)/V
            * ,EDQL(-,W,E),GETL #1
            * ,CHRO(I,/,#,R,N1,2,A>5,3,G-4,4,D-10,10,E)
            * ,EVALOK
            * ,LOOP
            *
            GETS
            LIBR  (I,',F,N-,X2,3,H,HS,J<1,E)/V
            EDQL  (-,W,E)
            GETL #1
            CHRO  (I,/,#,R,N1,2,A>5,3,G-4,4,D-10,10,E)
            EVALOK
               * ,[PART OF EVALO \ CAN WE HANDLE EDQL HERE? \]
               * ,IF '28 EVALOK,EVALOK
               * ,EDQL TEMP,EVAL(U*20,100,A;E)
               *
               IF EVALOK'28,EVALOK
               EDQL TEMP,EVAL (U*20,100,A,E)
            LOOP
         QUAN EVAL (I,H,E)
      EDSL $1 (-,'12,A,E)
      EDSL TEMP,$1 (A,E)
      EDSL TEMP (-,W,E)
      BEEP
   LOOP
FEED
BEEP
BEEP
BEEP
ERASE
```

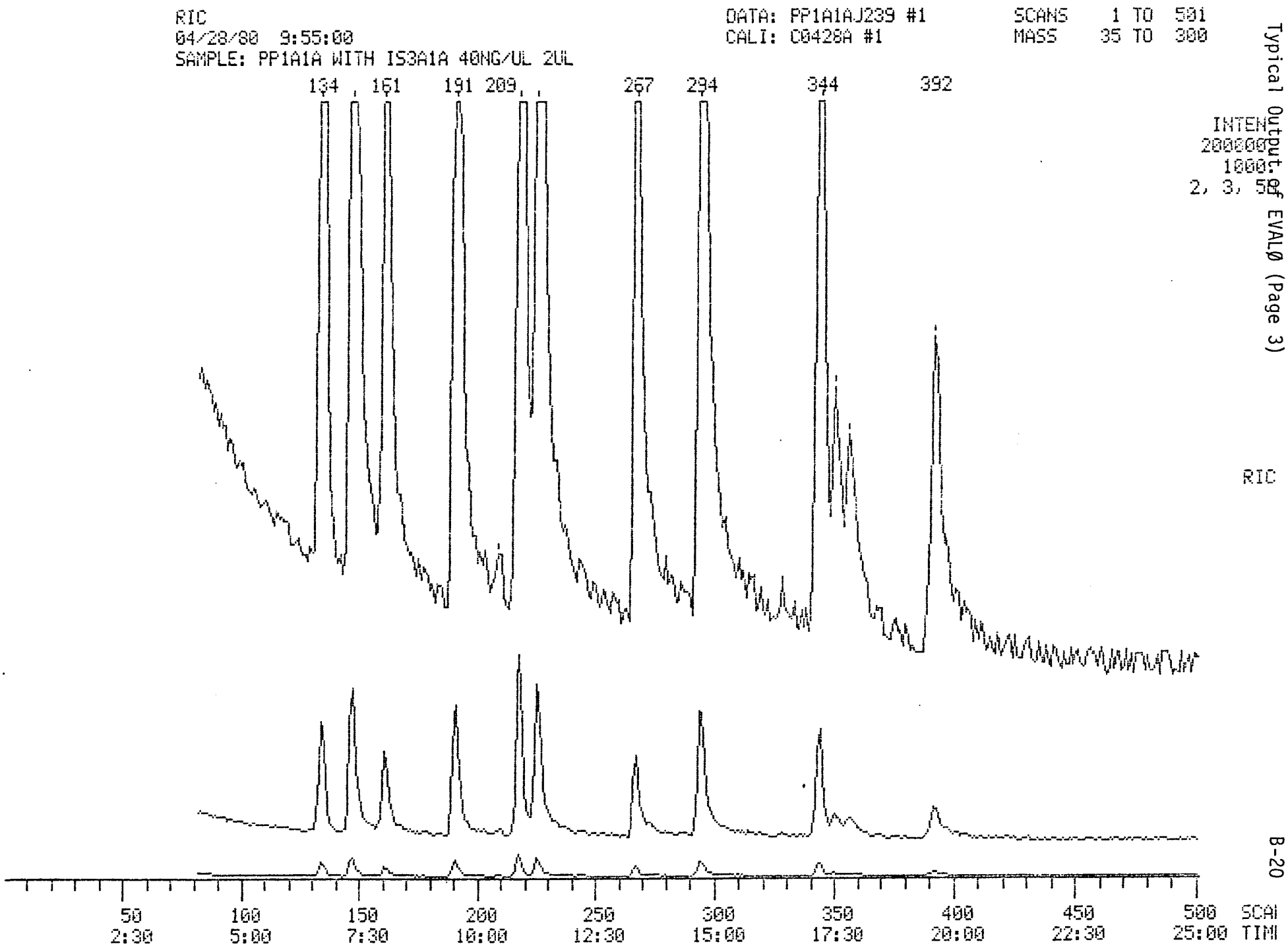
```
PRINP1.ME = C2;D;T;   IDENTIFICATION REPORT          FILE:
;$1;C2;T;NO   SCAN   PURITY   FIT
;C;E
```

```
PRINP2.ME = C20;T;                                    PRIORITY POLLUTANT EVALUATION
C;T;                    NO INTERNAL STANDARD WAS FOUND IN SAMPLE ;$1;
C;T;                                    ;D
;F;E
```

```
PRINNM.ME = T;U.S. ENVIRONMENTAL PROTECTION AGENCY
;C;T;NATIONAL ENFORCEMENT INVESTIGATIONS CENTER
;C;T;DENVER FEDERAL CENTER   BLDG 53 BOX 25227
;C;T;DENVER, CO 80225
;C2;E
```

```
PARAMETERS                    DATA: PP1A1AJ239 TI (PP1A1AJ239 MI)
04/28/80  9:55:00 + 30 36     CALI  C0428A              SCANS   79 TO  612
SAMPLE: PP1A1A WITH ISOA1A 40NG/UL 2UL
CONDS.: 70-190 8C/MIN
FORMULA:                      INSTRUMENT  3200EI        WEIGHT      0 000
SUBMITTED BY  JFC             ANALYST  JFC              ACCT  NO    J239

ACC. VOL..    8000            THRESHOLD        2        INTEN/ION         2
A/D S I :     0 025           CENT S.I..    0 200       FRAG S I      1.200
PEAK WIDTH:   1000            CENT SAMP/PK     56       FRAG SAMP/PK.     9
MIN. WIDTH:      2            MIN FRAG WIDTH (%): 80    MIN AREA         75

612 SCANS (355 SECTORS) OF LINEAR UP CENTROID DATA

LOW MASS:     35  SCAN TIMES (SECS ) UP:   2.95      TOP:   0.00
HIGH MASS.   300                      DOWN:   0 00   BOTTOM:  0 05

THERE IS A SCAN LIST WITH     0 ENTRIES

THERE IS A QUANTITATION LIST WITH  13 ENTRIES
```


RIC
04/28/80 9:55:00
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL
RANGE: G 79, 612 LABEL: N 0, 4.0 QUAN: A 0, 1.0 BASE: U 20, 3
DATA: PP1A1AJ239 #1
CALI: C0428A #1
SCANS 1 TO 612
100.0
RIC
550912
79
134
147
161
191
218
267
294
344
392
456
488
514
556
100
5:00
200
10:00
300
15:00
400
20:00
500
25:00
600
30:00
SCAN
TIME


RIC
04/28/80 9:55:00
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL
DATA: PP1A1AJ239 #1
CALI: C0428A #1
SCANS 1 TO 501
MASS 35 TO 300
134
161
191
209
267
294
344
392
INTEN
200000
1000.0
2, 3, 5
RIC
50
2:30
100
5:00
150
7:30
200
10:00
250
12:30
300
15:00
350
17:30
400
20:00
450
22:30
500
25:00
SCAN
TIME

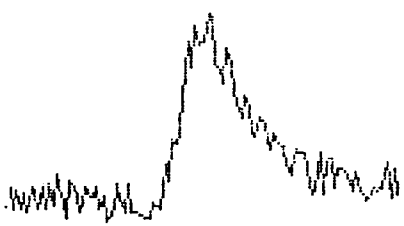
RIC
04/28/80 9:55:00
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL

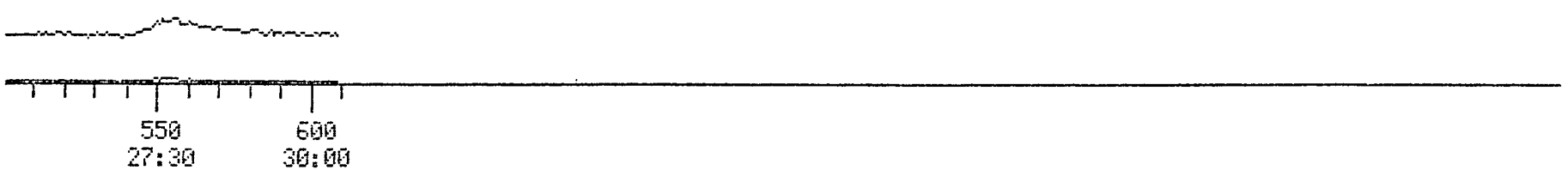
DATA: PP1A1AJ239 #1
CALI: C0428A #1

SCANS 501 TO 612
MASS 35 TO 300

INTEN
200000.
1000.
2, 3, 5N

RIC





SCAN
TIME

NAM	NUM:	WT	FORMULA	NAME
PP	133:	188	C14 D10	ISA D10-PHENANTHRENE (133)
PP	135·	136	C8. D8	ISA D8-NAPHTHALENE (135)
PP	21·	196	C6 H3 O. CL3	21 2,4,6-TRICHLOROPHENOL
PP	22	142	C7. H7 O CL	22 4-CHLORO-3-METHYLPHENOL
PP	24:	128	C6 H5. O. CL	24 2-CHLOROPHENOL
PP	31	162	C6. H4. O CL2	31 2,4-DICHLOROPHENOL
PP	34.	122	C8. H10. O	34 2,4-DIMETHYLPHENOL
PP	57:	139	C6 H5 O3. N	57 2-NITROPHENOL
PP	58	139	C6 H5 O3. N	58 4-NITROPHENOL
PP	59:	184	C6. H4 O5. N2	59 2,4-DINITROPHENOL
PP	60.	198	C7. H6 O5. N2	60 4,6-DINITRO-O-CRESOL
PP	64:	264	C6 H O. CL5	64 PENTACHLOROPHENOL
PP	65·	94	C6. H6. O	65A PHENOL
PP	134:	162	C7 H5 O F3	SUA A,A,A-TRIFLUORO-M-CRESOL (134)

5/27/80 17·30:04 IDENTIFICATION REPORT FILE· D.PP1A1AJ239.TI

NO	SCAN	PURITY	FIT
*1	344	732	968
*1	134	742	987
21	267	547	984
22	294	610	913
24	147	737	972
31	225	622	970
34	218	764	977
57	161	574	961
58	555	341	975
59	350	115	720
60	356	173	795
64	392	354	948
65	191	781	981
*1	225	164	538

QUANTITATION REPORT FILE: PP1A1AJ239

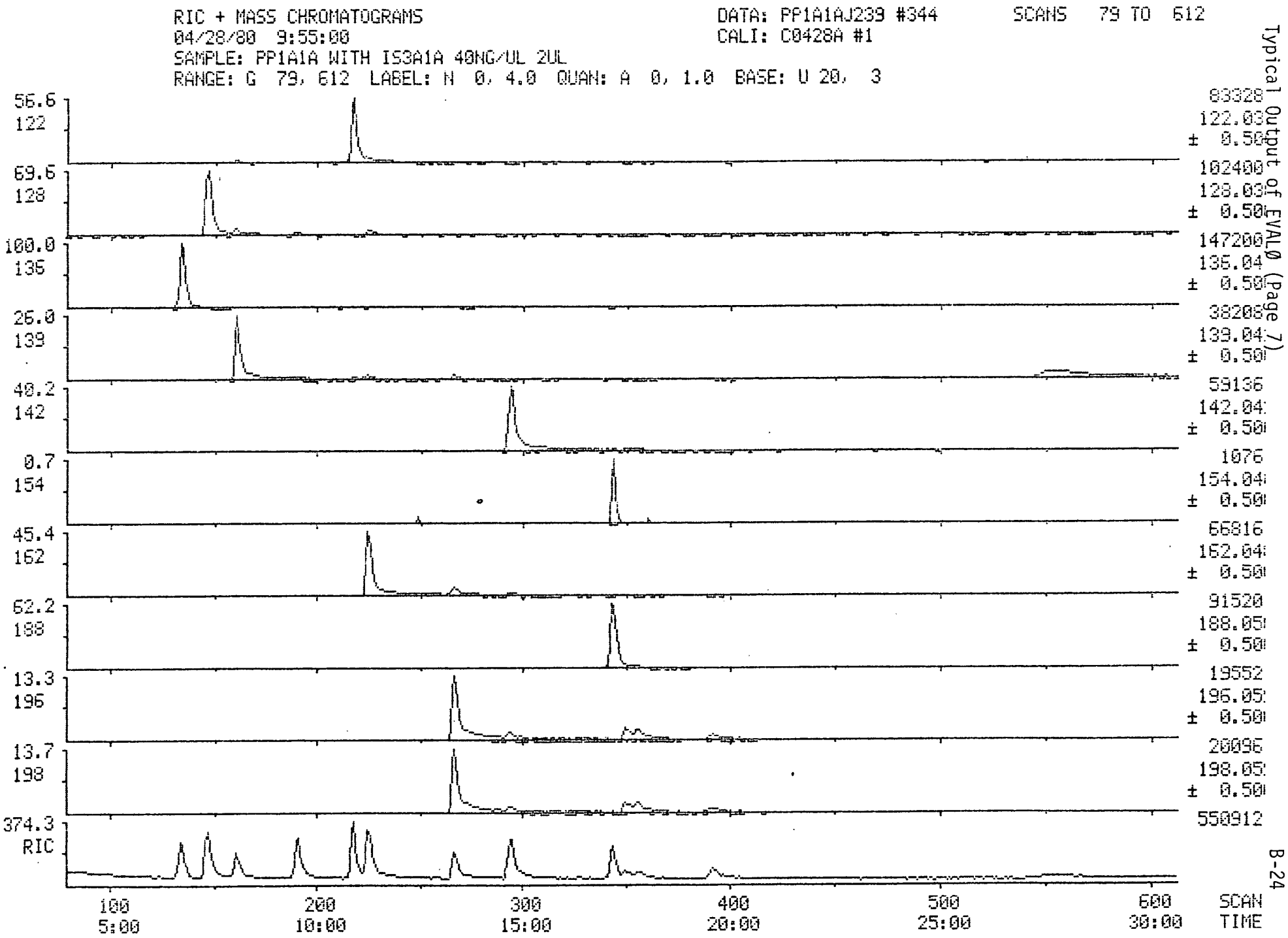
DATA: PP1A1AJ239 TI
04/28/80 9 55:00
SAMPLE. PP1A1A WITH IS3A1A 40NG/UL 2UL
CONDS. . 70-190 8C/MIN
FORMULA. INSTRUMENT 3200EI WEIGHT. 0 000
SUBMITTED BY JFC ANALYST JFC ACCT. NO J239

AMOUNT=AREA * REF AMNT/(REF AREA* RESP. FACT)

NO	NAME
1	ISA D10-PHENANTHRENE (133)
2	ISA D8-NAPHTHALENE (135)
3	21 2,4,6-TRICHLOROPHENOL
4	22 4-CHLORO-3-METHYLPHENOL
5	24 2-CHLOROPHENOL
6	31 2,4-DICHLOROPHENOL
7	34 2,4-DIMETHYLPHENOL
8	57 2-NITROPHENOL
9	58 4-NITROPHENOL
10	59 2,4-DINITROPHENOL
11	60 4,6-DINITRO-O-CRESOL
12	64 PENTACHLOROPHENOL
13	65A PHENOL
14	SUA A,A,A-TRIFLUORO-M-CRESOL (134)

NO	M/E	SCAN	TIME	REF	RRT	METH	AREA	AMOUNT	%TOT
1	188	343	17.09	1	1.000	A BB	336606.	40 000 NG/UL	2 67
2	136	134	6:42	1	0.391	A BB	486994.	40 000 NG/UL	2 67
3	196	267	13 21	1	0.778	A BB	66258.	100.000 NG/UL	6.68
4	142	294	14:42	1	0.857	A BB	211184.	100.000 NG/UL	6.68
5	128	147	7 21	1	0.429	A BB	374173.	100 000 NG/UL	6 68
6	162	225	11 15	1	0.656	A BB	220935.	100.000 NG/UL	6 68
7	122	218	10 54	1	0.636	A BB	271617.	100.000 NG/UL	6 68
8	139	161	8 03	1	0 469	A BB	115756.	100.000 NG/UL	6.68
9	139	554	27:42	1	1.615	A BB	22657.	417.500 NG/UL	27.88
10	NOT FOUND								
11	198	356	17 48	1	1.038	A VB	15153.	100.000 NG/UL	6.68
12	266	392	19 36	1	1.143	A BB	21734	200 000 NG/UL	13.36
13	94	191	9:33	1	0 557	A BB	449189.	100.000 NG/UL	6.68
14	NOT FOUND								

NO	RET(L)	RATIO	RRT(L)	RATIO	AMNT	AMNT(L)	R FAC	R FAC(L)	RATIO
1	17:09	1.00	1.000	1.00	40 00	40 00	1 000	1.000	1 00
2	6 42	1.00	0 391	1.00	40 00	40.00	1 447	1.447	1 00
3	13 21	1 00	0.778	1 00	100 00	100 00	0 079	0.079	1 00
4	14 42	1.00	0.857	1 00	100 00	100 00	0 251	0 251	1 00
5	7:21	1.00	0 429	1 00	100 00	100 00	0.445	0 445	1 00
6	11:15	1 00	0.656	1.00	100 00	100.00	0 263	0 262	1 00
7	10 54	1.00	0 636	1.00	100 00	100 00	0 323	0 323	1 00
8	8 03	1 00	0 469	1 00	100 00	100 00	0 138	0 138	1 00
9	27 42	1 00	1 615	1 00	417.50	400 00	0 007	0.006	1 04
10	17 57		1.034			200.00		0 009	
11	17:48	1.00	1.038	1 00	100.00	100.00	0 018	0 018	1.00
12	19.36	1 00	1.143	1 00	200 00	200 00	0 013	0 013	1 00
13	9:33	1.00	0.557	1 00	100 00	100 00	0 534	0.534	1 00
14	11 16		0 651			300 00		0 390	


RIC + MASS CHROMATOGRAMS
04/28/80 9:55:00
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL
RANGE: G 79, 612 LABEL: N 0, 4.0 QUAN: A 0, 1.0 BASE: U 20, 3
DATA: PP1A1AJ239 #344
CALI: C0428A #1
SCANS 79 TO 612
56.6
122
69.6
128
100.0
136
26.0
139
40.2
142
0.7
154
45.4
162
62.2
188
13.3
196
13.7
198
374.3
RIC
100
5:00
200
10:00
300
15:00
400
20:00
500
25:00
600
30:00
SCAN
TIME
Typical Output of EVAL0 (Page 7)
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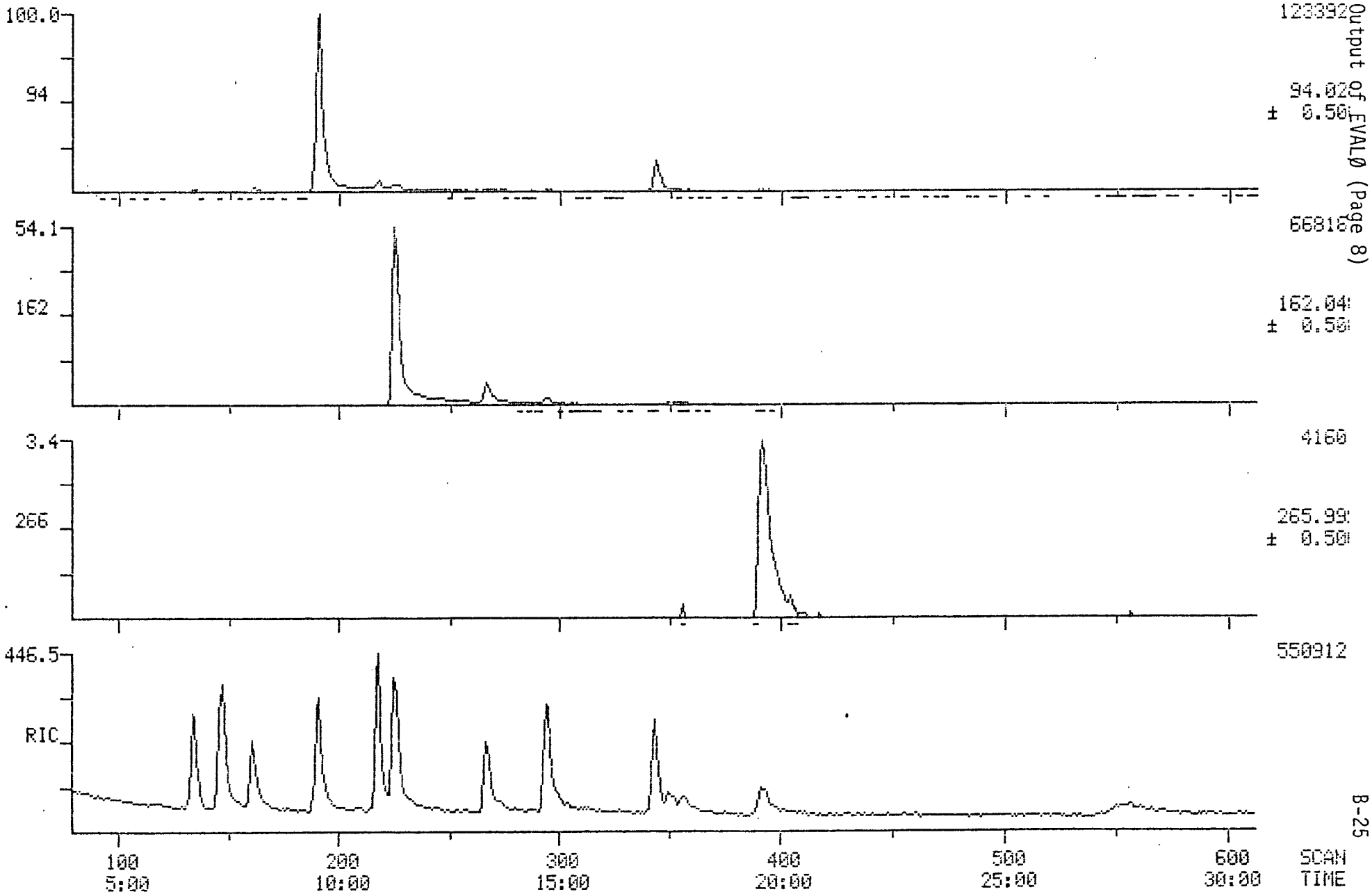

RIC + MASS CHROMATOGRAMS
04/28/80 9:55:00
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL
RANGE: G 79, 612 LABEL: N 0, 4.0 QUAN: A 0, 1.0 BASE: U 20, 3
DATA: PP1A1AJ239 #344
CALI: C0428A #1
SCANS 79 TO 612
100.0
94
123392
94.02
± 0.50
54.1
162
66816
162.04
± 0.50
3.4
266
4160
265.99
± 0.50
446.5
RIC
550912
100
5:00
200
10:00
300
15:00
400
20:00
500
25:00
600
30:00
SCAN
TIME

APPENDIX C

Operation of EVAL2

Procedure EVAL2

>EVAL2 LIBRARY LIST, YES or NO (NB Library Search), YES or NO (Print Target Compound Spectra) activates the procedure.

This procedure is similar in operation to EVALØ. The procedure is used to process data files stored on Unit #2 of a Two-Disk-Drive System. The data files to be evaluated are stored in namelist 2:EVAL.

```
>EDNL 2:EVAL
EDNL: N; FILENAME
EDNL: W;E
      or
>SETN 2: EVAL
>FILE
FILE: D2: FILENAME
FILE: >
Append file displayed to namelist EVAL stored on Unit #2.
```

The quantitation results are appended to a quantitation list stored on Unit #2. The library list must be stored on Unit #3. Copy the library list needed from Unit #1 to Unit #3.

```
TRACE OF PROCEDURE EVAL2
   ↓ ERASE
   * ,[PROCEDURE EVAL2 PR                                                    ]
   * ,[WRITTEN 9/4/79 BY O J LOGSDON II, LAST REVISION 04/21/8Ø BAH          ]
   * ,[US EPA/NATIONAL ENFORCEMENT INVESTIGATIONS CENTER 303-234-4661         ]
   * ,[                                                                      ]
   * ,[   TO PROCESS DATA ON DISC DRIVE UNIT 2, USE THIS PROCEDURE           ]
   * ,[  ****** YOU MUST COPY THE LIBRARY LIST OF INTEREST TO UNIT 3  ******  ]
   * ,[                                                                      ]
   * ,[  >EVAL2 LIBRARYLIST,YES OR NO (NB SEARCH)YES OR NO (PRINT SPECTRA)   ]
   * ,[   WHERE THE LIBRARYLIST CONTAINS AT A MINIMUM AN INTERNAL STANDARD,   ]
   * ,[         OTHER PEAKS SUCH AS PRIORITY POLLUTANTS MAY BE INCLUDED FOR   ]
   * ,[         QUANTITATION AND IDENTIFICATION   NB SEARCH OF ANY LABELED BUT]
   * ,[         UNIDENTIFIED PEAKS DURING THE QUANTITATION MAY BE SELECTED    ]
   * ,[         ALSO, PRINTOUT OF THE IDENTIFIED SPECTRA FROM THE QUANTITATION]
   * ,[         RUN MAY BE SUPRESSED WITH A 'NO' RESPONSE ('YES' REQUIRED     ]
   * ;[         OTHERWISE)                                                    ]
   * ,SETQ 2·TEMP
   * ,EDNL 2 EVTEMP (-,$3,$2,$1,W,E)
   * ;EDSL 2.TEMP(-,W,E)
   * ,EDSL 2.YES (-,1,W,E); EDSL 2 NO (-,W,E)
   * ,SET11 #0
   * ,SET12 #0
   * ,EVAL2A
   * ,FEED,BEEP,BEEP,BEEP
   * ,ERASE,[PROCEDURE EVAL2 IS DONE]
   *
   ERASE
   SETQ 2·TEMP
   EDNL 2 EVTEMP (-,$3;$2,$1,W,E)
   EDSL 2 TEMP (-,W,E)
   EDSL 2:YES (-,1,W,E)
   EDSL 2 NO (-,W,E)
   SET11
   SET12
   EVAL2A
      * ,[ PART OF EVAL2 \MAIN PROCESSING LOOP\ ]
      * ;SETN 2 EVAL,SET5 '11;GETN,SET11 '5
      * ,EDLL 2 $1(-,W,E)
      * ,EVAL2B
      * ,LOOP
      *
      SETN 2 EVAL
      SET5 !11
      GETN
      SET11 '5
      EDLL 2 $1 (-,W,E)
      EVAL2B
         * ,[ PART OF EVAL2 \SETUP AND PROCESSING\ ]
         * ,PARA(I,H,E)
         * ,CHRO(H1,2ØØØ,E)
         * ,SETS 2.$1,EDSL(-,W,E)
         * ,FILE(K PRIN 99/N,E),EDQL 2 $1 (-,W,E)
         * ,MAP(I,F1,U1ØØØ,V2ØØØØØ,35,300,N>2,3,5,H1,2ØØØ,500,E)
         * ,SET3 $1,SETN 2 EVTEMP,GETN #3,SETL 3 $1#Ø,GETN #1,SETS 2 $1,SET1 $3
         * ,EVAL2C
         * ,EVAL2D
         * ,EDLL (B'1,E)
         * ,PRIN(@P1),FILE(C PRIN 99,M /N,E),FEED
         * ,QUAN 2 $1(I,F2,H,E)
         * ,EVALMO
         * ,SET3 $1,SETN 2 EVTEMP,GETN #2,SETS 2 $1,SET1 $3
```

```
* ,EVAL2E
* ,EDSL 2 $1(-,'12,A,E)
* ,EDSL 2 TEMP,2 $1(A,E)
* ,EDSL 2 TEMP(-,W,E)
* ,BEEP
*
PARA  (I,H,E)
CHRO  (H1,2000,E)
SETS 2 $1
EDSL  (-,W,E)
FILE  (K PRIN 99/N,E)
EDQL 2 $1 (-,W,E)
MAP   (I,F1,U1000,V2000000,35,300,N>2,3,5,H1,2000,500,E)
SET3 $1
SETN 2 EVTEMP
GETN #3
SETL 3 $1
GETN #1
SETS 2 $1
SET1 $3
EVAL2C
   * ,[ PART OF EVAL2 \LOCATE INTERNAL STD\ ]
   * ,SET14 #0
   * ,GETL
   * ,SEAR/V(I,$,&,V4000000,N2,10,500,D-25,25,E)
   * ,EVAL2F
   * ,SET10 '14,SETL #0
   *
   SET14
   GETL
   SEAR  (I,$,&,V4000000,N2,10,500,D-25,25,E)/V
   EVAL2F
      * ,[ PART OF EVAL2 \ ?? INT  STD FOUND ?? \ ]
      * ,IF EVAL2F#1,'14
      * ;PRIN(@P2),BEEP,BEEP;BEEP,BEEP
      * ;RETU EVAL2B
      *
      IF EVAL2F#1,!14
      PRIN  (@P2)
      BEEP
      BEEP
      BEEP
      BEEP
      RETU EVAL2B
   SET10 '14
   SETL
EVAL2D
   * ,[ PART OF EVAL2 \DETECT SELECTED COMPOUNDS \ ]
   * ,SET1 '10,SET14 #0
   * ,GETL
   * ,SEAR/V(I,$,%,V4000000,N1,10,10,D-10,10,E)
   * ,PRIN/KX('4,2,'14,6,'15,6,'16,6,C,E)
   * ,EVAL2G
   * ,LOOP
   *
   SET1 '10
   SET14
   GETL
   SEAR  (I,$,%,V4000000,N1,10,10,D-10,10,E)/V
   PRIN  ('4,2,'14,6,'15,6,'16,6,C,E)/KX
   EVAL2G
      * ,[ PART OF EVAL2 \QUANT LOOP ENTRY\ ]
      * ,EVAL2H,EDQL 2 $1(-,N,#,A,E)
      *
      EVAL2H
         * ,[ PART OF EVAL2 \MATCH CHECK AND QUANT\ ]
```

```
          * ,[CHANGE THE NUMBER '#800' TO DESIRED LEVEL OF COMPUTER MATCH]
          * ,IF EVAL2H '16,EVAL2H #800
          * ,SET1 '14
          * ,EDSL 2 TEMP(-,'14,A,E)
          * ,EDLL 2 $1(-,$,A,E)
          * ,EDQL(-,W,E)
          * ,CHRO(I,R,$,#,N1,2,A>5,3,G-4,4,D-10,10,E)
          * ,EVAL2I,RETU EVAL2G
          *
          IF EVAL2H'16,EVAL2H#800
          SET1 '14
          EDSL 2 TEMP (-,'14,A,E)
          EDLL 2 $1 (-,$,A,E)
          EDQL  (-,W,E)
          CHRO  (I,R,$,#,N1,2,A>5,3,G-4,4,D-10,10,E)
          EVAL2I
             * ,[ PART OF EVAL2 \SPECTRUM PRINTOUT\ ]
             * ,IF EVAL2H '28,EVAL2H
             * ,EDQL 2 TEMP,2 $1(U*20,100,A,E)
             * ,EDSL 2 $1(I,-'1,4,W,E)
             * ,IF EVAL2I '27,EVAL2I
             * ,LIBR(',I,N-,C,DS,HS,E)
             *
             IF EVAL2H'28,EVAL2H
             EDQL 2 TEMP,2 $1 (U*20,100,A,E)
             EDSL 2 $1 (I,-'1,4,W,E)
             IF EVAL2I'27,EVAL2I
             LIBR  (',I,N-,C,DS,HS,E)
          RETU EVAL2G
       EDQL 2 $1 (-;N,#,A,E)
    LOOP
EDLL  (B'1,E)
PRIN  (@P1)
FILE  (C PRIN 99,M /N,E)
FEED
QUAN 2 $1 (I,F2,H,E)
EVALM0
    * SETL #0,SET10 #0
    * ,EVALM1
    * ,CHRO(H,I;E)
    *
    SETL
    SET10
    EVALM1
       * GETL
       * ,CHRO($,K,E)
       * ,EVALM2
       * ,LOOP
       *
       GETL
       CHRO  ($,K,E)
       EVALM2
          * SET10 '10#1
          * ,IF '10 EVALM2,#10
          * ,CHRO(H,I,E)
          * ;SET10 #0
          *
          SET10 #1'10
          IF EVALM2'10,#10
          CHRO  (H,I,E)
          SET10
       LOOP
    CHRO  (H,I,E)
 SET3 $1
 SETN 2 EVTEMP
 GETN #2
```

```
      SETS 2 $1
      SET1 $3
      EVAL2E
         * ,[ PART OF EVAL2 \SELECT 'NB' SEARCH?\ ]
         * ,IF EVAL2E '27,EVAL2E
         * ,SET4 NB,SETL 2 TEMP,EDGL 2 $1,2 EVAL(I,-2,1000,W,E),SETS 2 $1
         * ,EVAL2J
         * ,QUAN 2 EVAL (I,H,E)
         *
         IF EVAL2E'27,EVAL2E
         SET4 NB
         SETL 2 TEMP
         EDGL 2 $1,2 EVAL (I,-2,1000,W,E)
         SETS 2 $1
         EVAL2J
            * ,[ PART OF EVAL2 \'NB' SEARCH LOOP\ ]
            * ,GETS
            * ,LIBR(I,',F,N-,X2,3,HS,J<1,E)/V
            * ,EDGL(-,W,E),GETL #1
            * ,CHRO(I,/,#,R,N1,2,A>5,3,G-4,4,D-10,10,E)
            * ,EVAL2K
            * ,LOOP
            *
            GETS
            LIBR  (I,',F,N-,X2,3,HS,J<1,E)/V
            EDGL  (-,W,E)
            GETL #1
            CHRO  (I,/,#,R,N1,2,A>5,3,G-4,4,D-10,10,E)
            EVAL2K
               * ,[PART OF EVAL2 \ CAN WE HANDLE EDGL HERE? \]
               * ,IF '28 EVAL2K,EVAL2K
               * ,EDGL 2 TEMP,2 EVAL(U*20,100,A,E)
               *
               IF EVAL2K'28,EVAL2K
               EDGL 2.TEMP,2 EVAL (U*20,100,A,E)
            LOOP
         QUAN 2 EVAL (I,H,E)
      EDSL 2 $1 (-,'12,A,E)
      EDSL 2 TEMP,2 $1 (A;E)
      EDSL 2 TEMP (-,W,E)
      BEEP
   LOOP
FEED
BEEP
BEEP
BEEP
ERASE
```

```
PRINP1.ME = C2;D;T;   IDENTIFICATION REPORT          FILE:
;$1;C2;T;NO   SCAN   PURITY   FIT
;C;E
```

```
PRINP2.ME = C20;T;                          PRIORITY POLLUTANT EVALUATION;
C;T;                NO INTERNAL STANDARD WAS FOUND IN SAMPLE ;$1;
C;T;                              ;D
;F;E
```

```
PRINNM.ME = T;U.S. ENVIRONMENTAL PROTECTION AGENCY
;C;T;NATIONAL ENFORCEMENT INVESTIGATIONS CENTER
;C;T;DENVER FEDERAL CENTER   BLDG 53 BOX 25227
;C;T;DENVER, CO 80225
;C2;E
```

APPENDIX D

Operation of Procedure ESPEC

Procedure ESPEC

Typical Output of ESPEC

>ESPEC YES or NO (NB Library Search) activates the procedure.

This procedure permits the delayed printing of the spectra of target compounds detected in a sample file and a delayed NBS Library search for non-target (unknown) compounds detected.

>EVALØ LIBRARY LIST, NO, NO

establishes delayed spectra printing and delayed identification of unknown compounds as an option by generating a scan list and a library list of the target compounds detected and a scan list of the non-target (unknown) compounds detected. The scan list and the library list are stored under the name of the filename used to generate the lists. Files to be processed using ESPEC are stored in namelist Ø:EVAL.

>ESPEC YES

outputs a scan list, library list, a comparison of the sample spectra to the target compound spectra stored in the user library, a comparison of each unknown spectrum to the three best spectral matches found in the NBS library for that compound, and a quantitation report indicating the best identifications of the unknown compounds found in the NBS library.

>ESPEC NO

outputs a scan list, library list, and a comparison of the sample spectra to the target compound spectra stored in the user library.

```
TRACE OF PROCEDURE ESPEC
   * ;ERASE
   * ;[ PROCEDURE ESPEC                                                    ]
   * ;[ ESPEC YES OR NO (NB LIBRARY SEARCH)  IS THE COMMAND THAT           ]
   * ,[ INITIATES EXECUTION OF THE PROCEDURE                               ]
   * ,[                                                                    ]
   * ;[ WRITTEN BY DA HUGHES  APRIL,1980  LAST REVISION 04/13/80 DAH       ]
   * ;[ US EPA-NEIC  303-234-4661                                          ]
   * ;[                                                                    ]
   * ;[ SAMPLE FILES TO BE PROCESSED MUST BE STORED ON DISC DRIVE          ]
   * ;[ UNIT#0.                                                            ]
   * ,[                                                                    ]
   * ;[ THIS PROCEDURE PERMITS THE DELAYED PRINTING OF THE SPECTRA OF      ]
   * ;[ PRIORITY POLLUTANTS DETECTED IN A SAMPLE FILE AND A DELAYED        ]
   * ;[ NB LIBRARY SEARCH FOR NON-PRORITY POLLUTANTS DETECTED  EVALO       ]
   * ;[ GENERATES A SCAN LIST AND A LIBRARY LIST OF THE PRIORITY           ]
   * ;[ POLLUTANTS DETECTED AND A SCAN LIST OF THE NON-PRIORITY            ]
   * ;[ POLLUTANTS DETECTED.                                               ]
   * ,[                                                                    ]
   * ;SET11 #0
   * ;SETQ TEMP
   * ;EDNL ETEMP (-;$1,W,E)
   * ;EDSL YES (-,1;W.E)
   * ;EDSL NO (-;W;E)
   * ;ESPEC1
   * ;FEED
   * ;BEEP
   *
   ERASE
   SET11
   SETQ TEMP
   EDNL ETEMP (-;$1:W,E)
   EDSL YES (-,1;W,E)
   EDSL NO (-,W;E)
   ESPEC1
      * ;SETN EVAL
      * ,SET5 !11
      * ;GETN
      * ;SET11 !5
      * ,ESPEC2
      * ;LOOP .
      *
      SETN EVAL
      SET5 !11
      GETN
      SET11 !5
      ESPEC2
         * ,[ PART OF ESPEC  \SETUP AND PROCESSING\]
         * ,PRIN (@E1)
         * ;SETS $1#0
         * ,EDSL $1(H,E)
         * ,ESPEC3
         * .SETL $1#0
         * ,EDLL $1(H,E)
         * ;ESPEC4
         * .SET3 $1
         * ;SETN ETEMP
         * ;GETN #1
         * ;SETS $1
         * ;SET1 $0
         * ,ESPEC5
         *
```

```
PRIN  (@E1)
SETS $1
EDSL $1 (H,E)
ESPEC3
   * ,[ PART OF ESPEC  \FIND THE DELIMETER BETWEEN UNK SCAN#'S ,PP SCAN#'S
   * ,GETS
   * ,IF ESPEC3'1,ESPEC3
   * ,LOOP
   *
   GETS
   IF ESPEC3'1,ESPEC3
   LOOP
SETL $1
EDLL $1 (H,E)
ESPEC4
   * ,[ PARTOF ESPEC  \PROCESS PP SCANS\ ]
   * ,GETS
   * ,GETL
   * ,LIBR(',I,N-,C,DS,HS,E)
   * ,LOOP
   *
   GETS
   GETL
   LIBR  (',I,N-,C,DS,HS,E)
   LOOP
SET3 $1
SETN ETEMP
GETN #1
SETS $1
SET1 $3
ESPEC5
   * ,[ PART OF EVALO AND ESPEC   \SELECT 'NB' SEARCH?\ ]
   * ;IF ESPEC5 '27,ESPEC5
   * ,PRIN (@E2)
   * ,SET4 NB,SETL TEMP,EDGL $1,EVAL(I,-2,1000,W,E),SETS $1
   * ,ESPEC6
   * ;QUAN EVAL (I,H,E)
   *
   IF ESPEC5'27,ESPEC5
   PRIN  (@E2)
   SET4 NB
   SETL TEMP
   EDGL $1,EVAL (I,-2,1000,W,E)
   SETS $1
   ESPEC6
      * ,[ PART OF EVALO AND ESPEC   \'NB' SEARCH LOOP\ ]
      * ,GETS
      * ,IF ESPEC6'1,ESPEC6
      * ,LIBR(I,',F,N-,X2,3,H,HS,J<1,E)/V
      * ,EDGL(-,W,E),GETL #1
      * ,CHRO(I,/,#;R,N1,2,A>5,3,G-4,4,D-10,10,E)
      * ,ESPEC7
      * ,LOOP
      *
      GETS
      IF ESPEC6'1,ESPEC6
      LIBR  (I,',F,N-,X2,3,H,HS,J<1,E)/V
      EDGL  (-;W,E)
      GETL #1
      CHRO  (I,/,#,R,N1,2,A>5,3,G-4,4,D-10,10,E)
      ESPEC7
         * ,[PART OF EVALO AND ESPEC   \ CAN WE HANDLE EDGL HERE? \]
         * ,IF '28 ESPEC7,ESPEC7
         * ,EDGL TEMP,EVAL(U*20,100,A,E)
         *
         IF ESPEC7'28,ESPEC7
```

```
                EDQL TEMP,EVAL (U*20,100,A,E)
             LOOP
          QUAN EVAL (I,H,E)
   LOOP
FEED
BEEP
```

```
PRINE1.ME = C10;T;PRIORITY POLLUTANT EVALUATION
;C;T;FILE:
$1;C;T;SPECTRA PRINTOUT
;C10;E
```

```
PRINE2.ME = C20;T;NB LIBRARY SEARCH
;C;T;FILE:
$1;C;T;SPECTRA PRINTOUT AND QUANTITATION REPORT
;F;E
```

```
PRINNM.ME = T;U.S. ENVIRONMENTAL PROTECTION AGENCY
;C;T;NATIONAL ENFORCEMENT INVESTIGATIONS CENTER
;C;T;DENVER FEDERAL CENTER   BLDG 53 BOX 25227
;C;T;DENVER, CO  80225
;C2;E
```

U.S. ENVIRONMENTAL PROTECTION AGENCY
NATIONAL ENFORCEMENT INVESTIGATIONS CENTER
DENVER FEDERAL CENTER BLDG 53 BOX 25227
DENVER, CO 80225

PRIORITY POLLUTANT EVALUATION
FILE: 0:PP1A1AJ239. TI
SPECTRA PRINTOUT

INPUT FILE: PP1A1AJ239. SL, OUTPUT FILE: PP1A1AJ239. SL

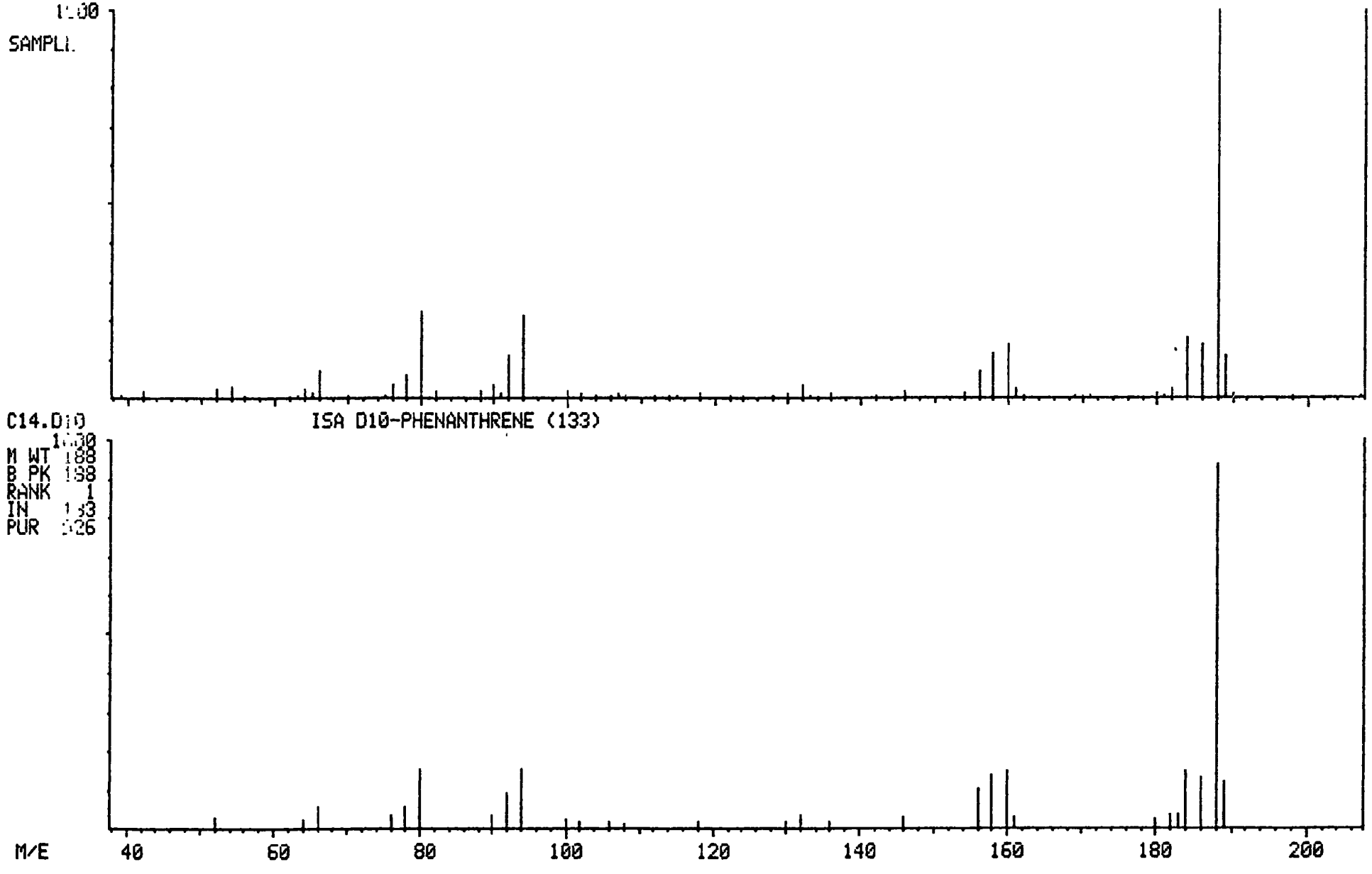
209	350	356	0	344	134	267	294	147	225	218	161
555	392	191									

```
INPUT FILE:  PP1A1AJ239.LL,  OUTPUT FILE:  PP1A1AJ239.LL
PP,   133   PP,   135   PP,   21   PP,   22   PP,   24   PP,   31
PP,    34   PP,    57   PP,   58   PP,   64   PP,   65
```

LIBRARY SEARCH
04/28/80 9:55:00 + 17:12
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL
ENHANCED (S 15B 2N 0T)

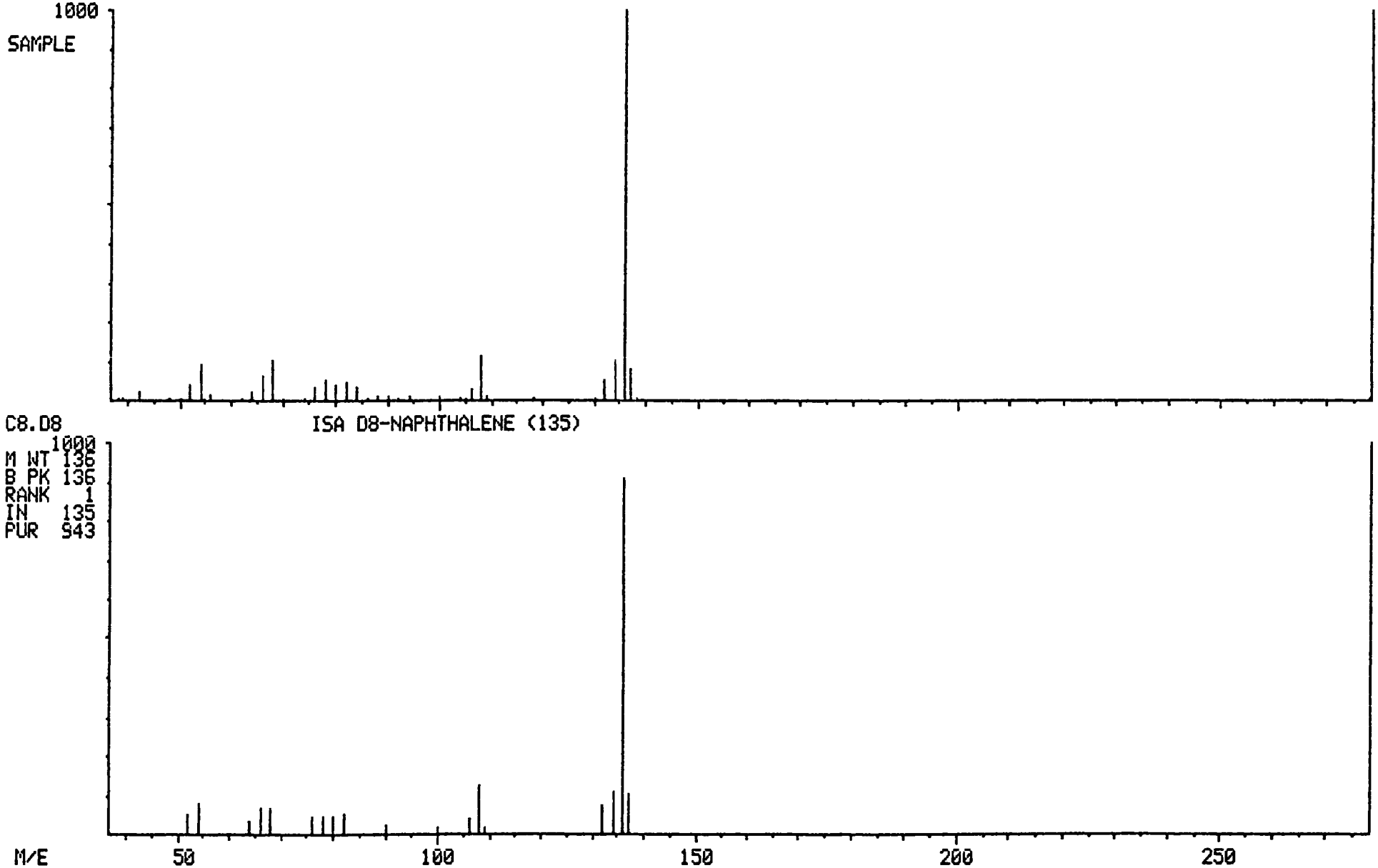
DATA: PP1A1AJ239 # 344
CALI: C0428A # 1

BASE M/E: 188
RIC: 258303.



LIBRARY SEARCH
04/28/80 9:55:00 + 6:42
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL
ENHANCED (S 15B 2N 0T)

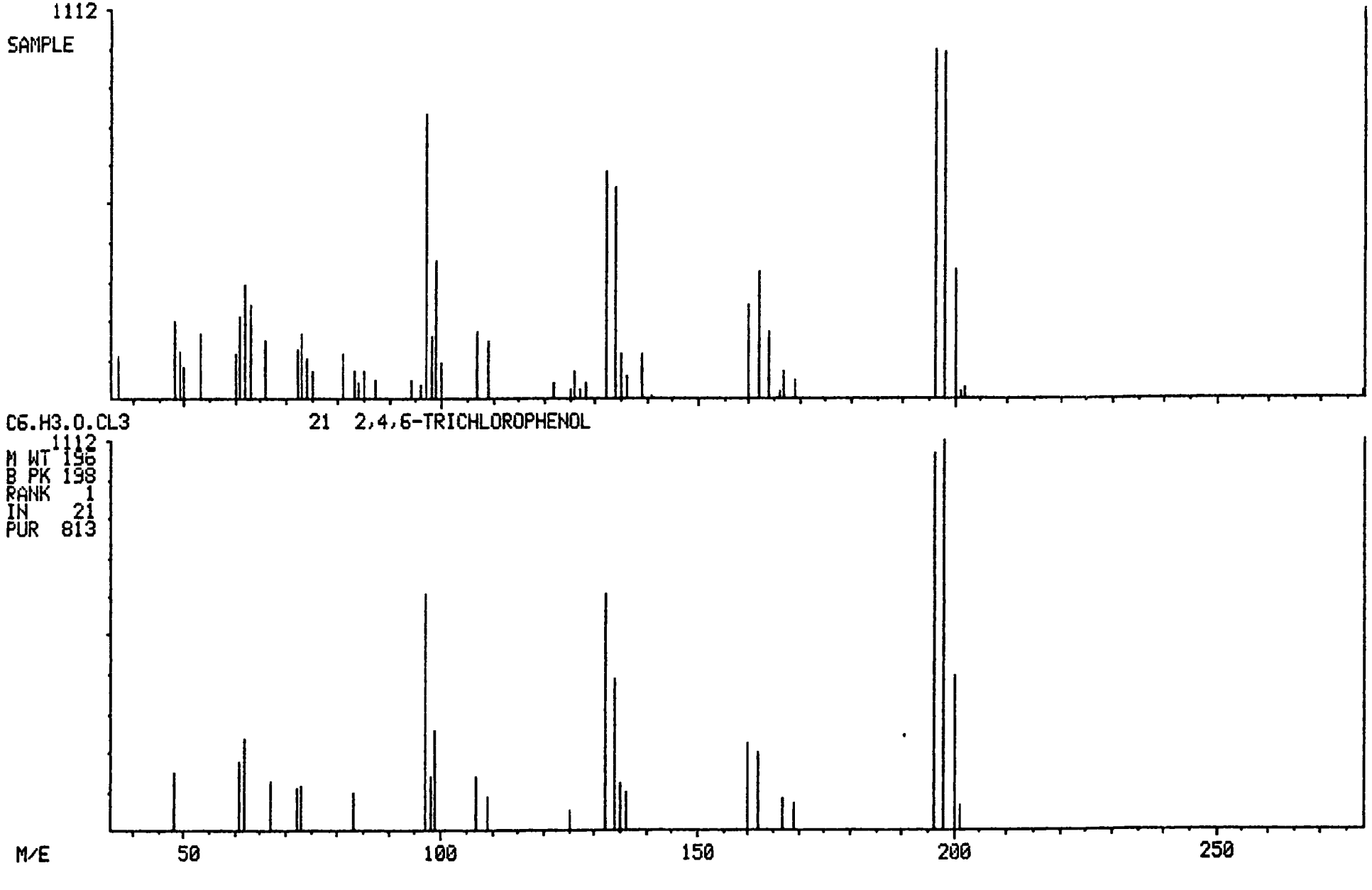
DATA: PP1A1AJ239 # 134 BASE M/E: 136
CALI: C0428A # 1 RIC: 276991.

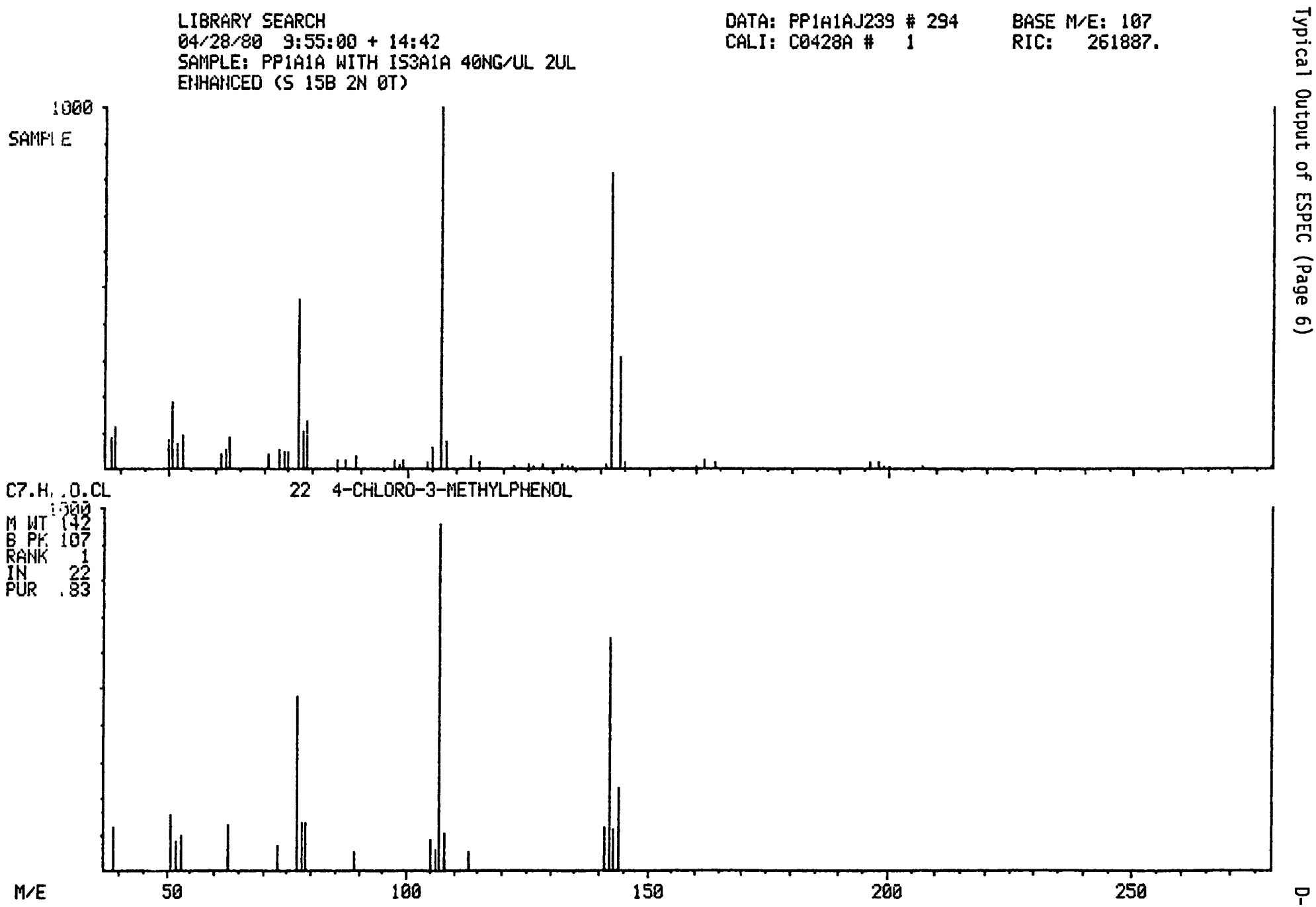


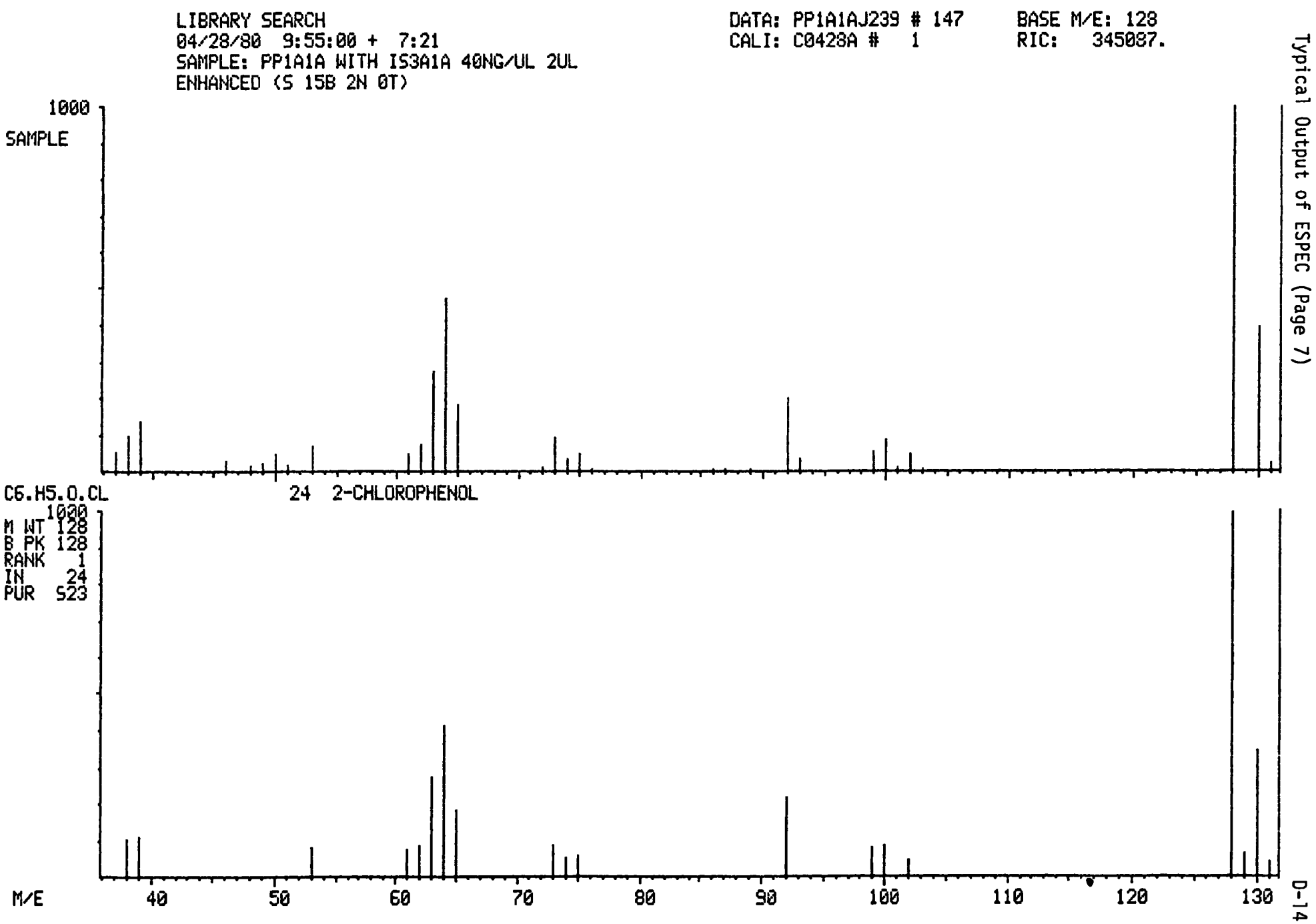
LIBRARY SEARCH
04/28/80 9:55:00 + 13:21
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL
ENHANCED (S 15B 2N 0T)

DATA: PP1A1AJ239 # 267
CALI: C0428A # 1

BASE M/E: 196
RIC: 166143.



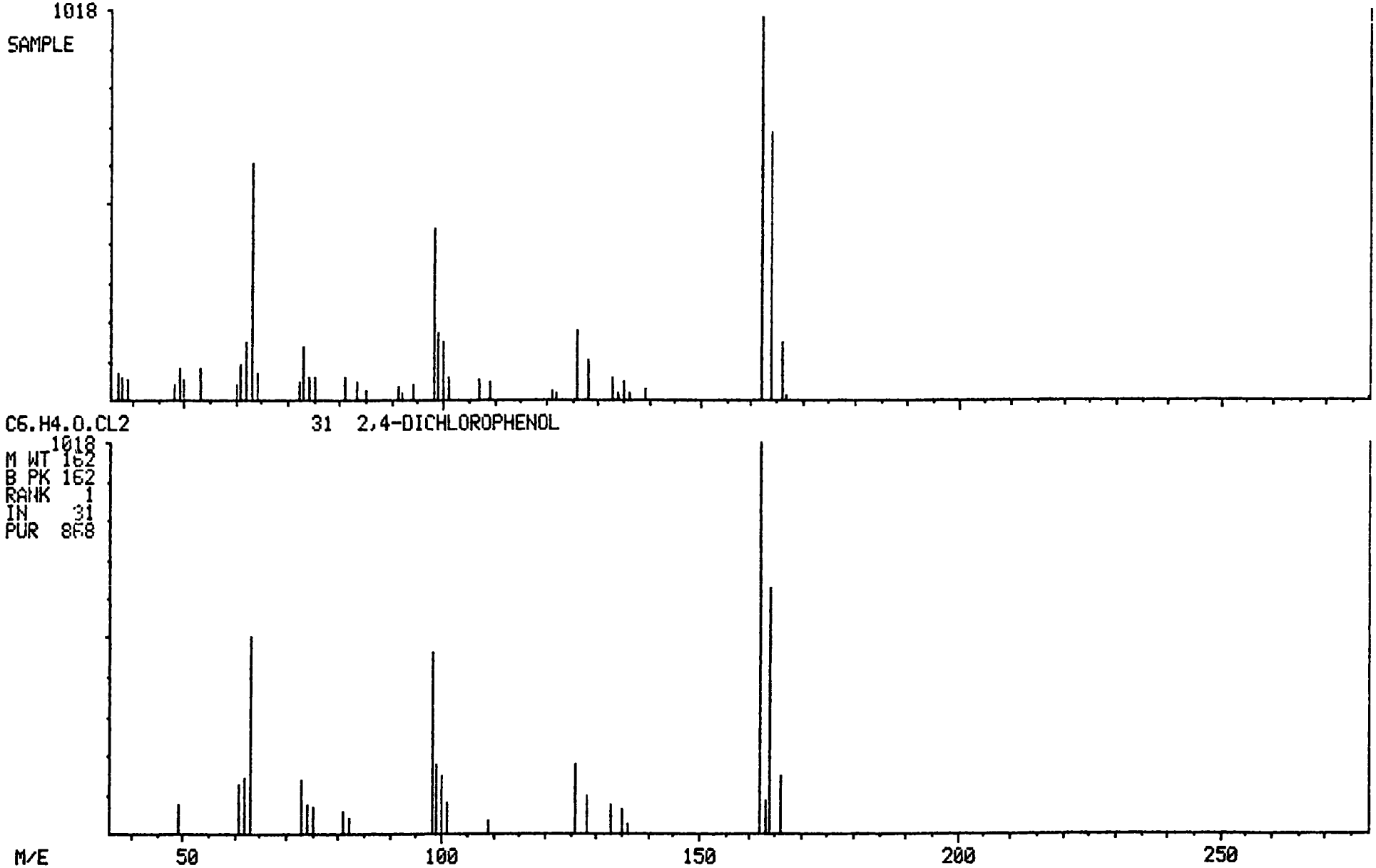

LIBRARY SEARCH
04/28/80 9:55:00 + 14:42
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL
ENHANCED (S 15B 2N 0T)
DATA: PP1A1AJ239 # 294
CALI: C0428A # 1
BASE M/E: 107
RIC: 261887.
1000
SAMPLE
C7.H..O.CL
22 4-CHLORO-3-METHYLPHENOL
1000
M WT 142
B PK 107
RANK 1
IN 22
PUR .83
M/E
50
100
150
200
250


LIBRARY SEARCH
04/28/80 9:55:00 + 7:21
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL
ENHANCED (S 15B 2N 0T)
DATA: PP1A1AJ239 # 147
CALI: C0428A # 1
BASE M/E: 128
RIC: 345087.
1000
SAMPLE
C6.H5.O.CL
24 2-CHLOROPHENOL
1000
M WT 128
B PK 128
RANK 1
IN 24
PUR 923
M/E
40
50
60
70
80
90
100
110
120
130

LIBRARY SEARCH
04/28/80 9:55:00 + 11:15
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL
ENHANCED (S 15B 2N 0T)

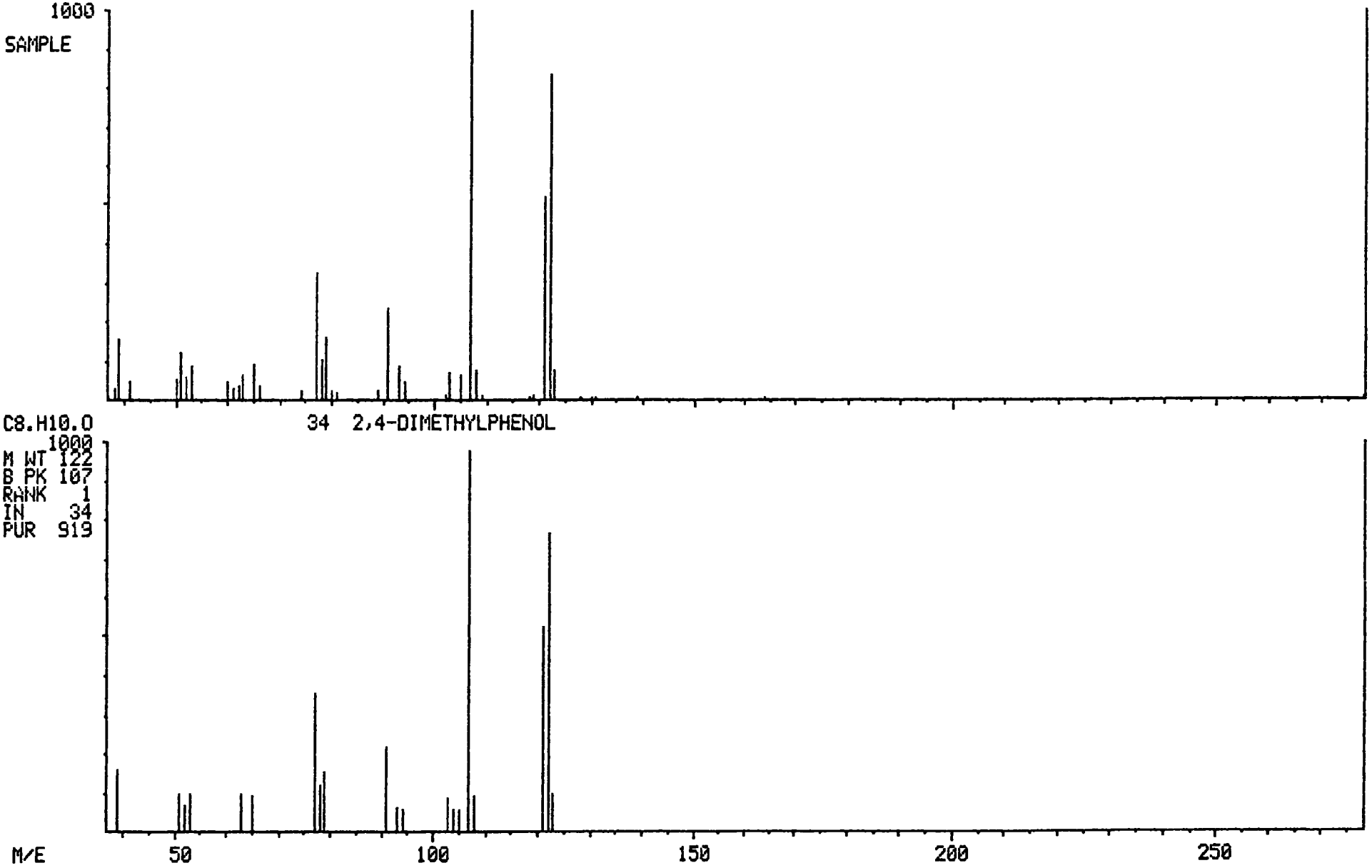
DATA: PP1A1AJ239 # 225
CALI: C0428A # 1

BASE M/E: 162
RIC: 300031.



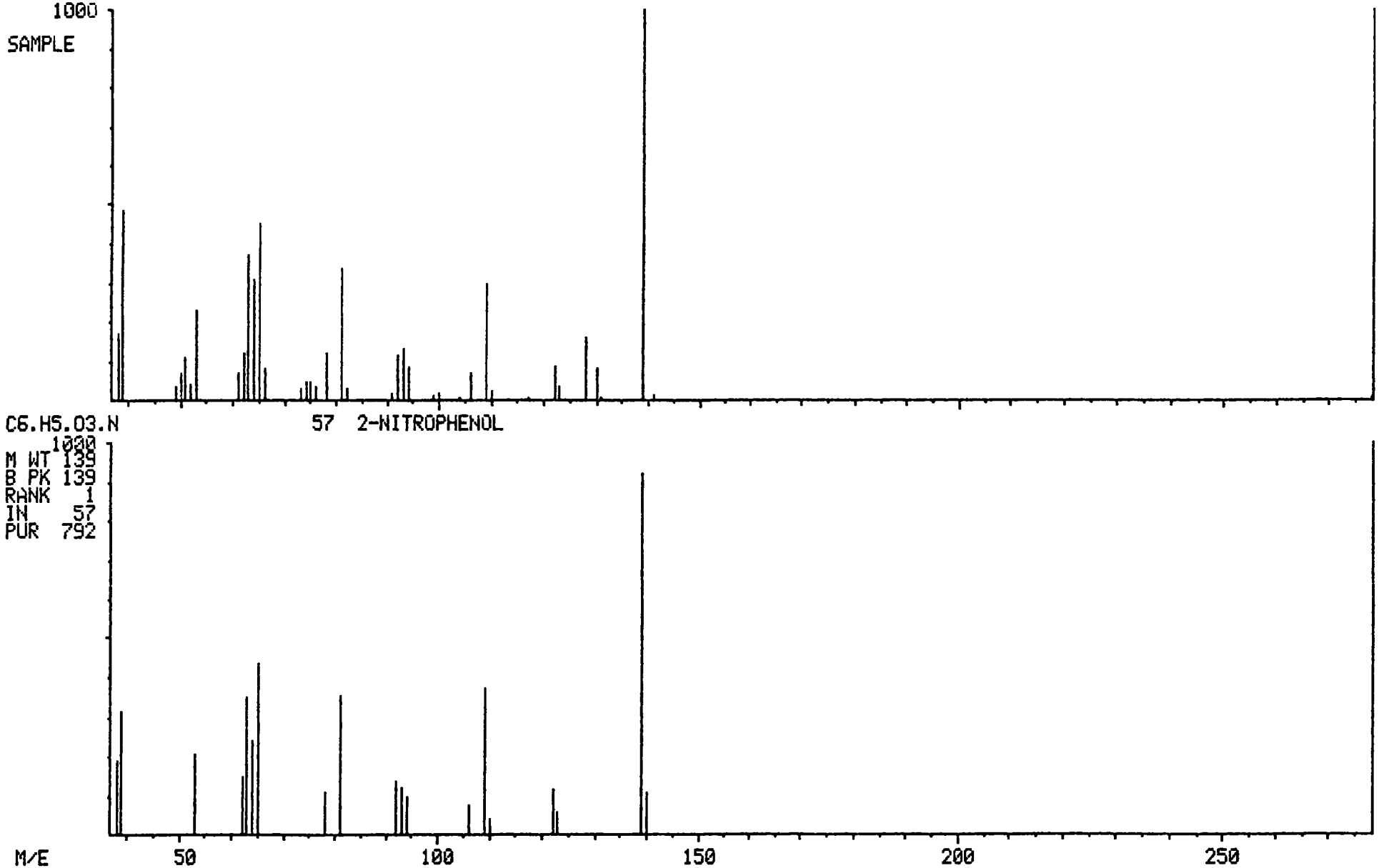
LIBRARY SEARCH
04/28/80 9:55:00 + 10:54
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL
ENHANCED (S 15B 2N 0T)

DATA: PP1A1AJ239 # 218 BASE M/E: 107
CALI: C0428A # 1 RIC: 409599.



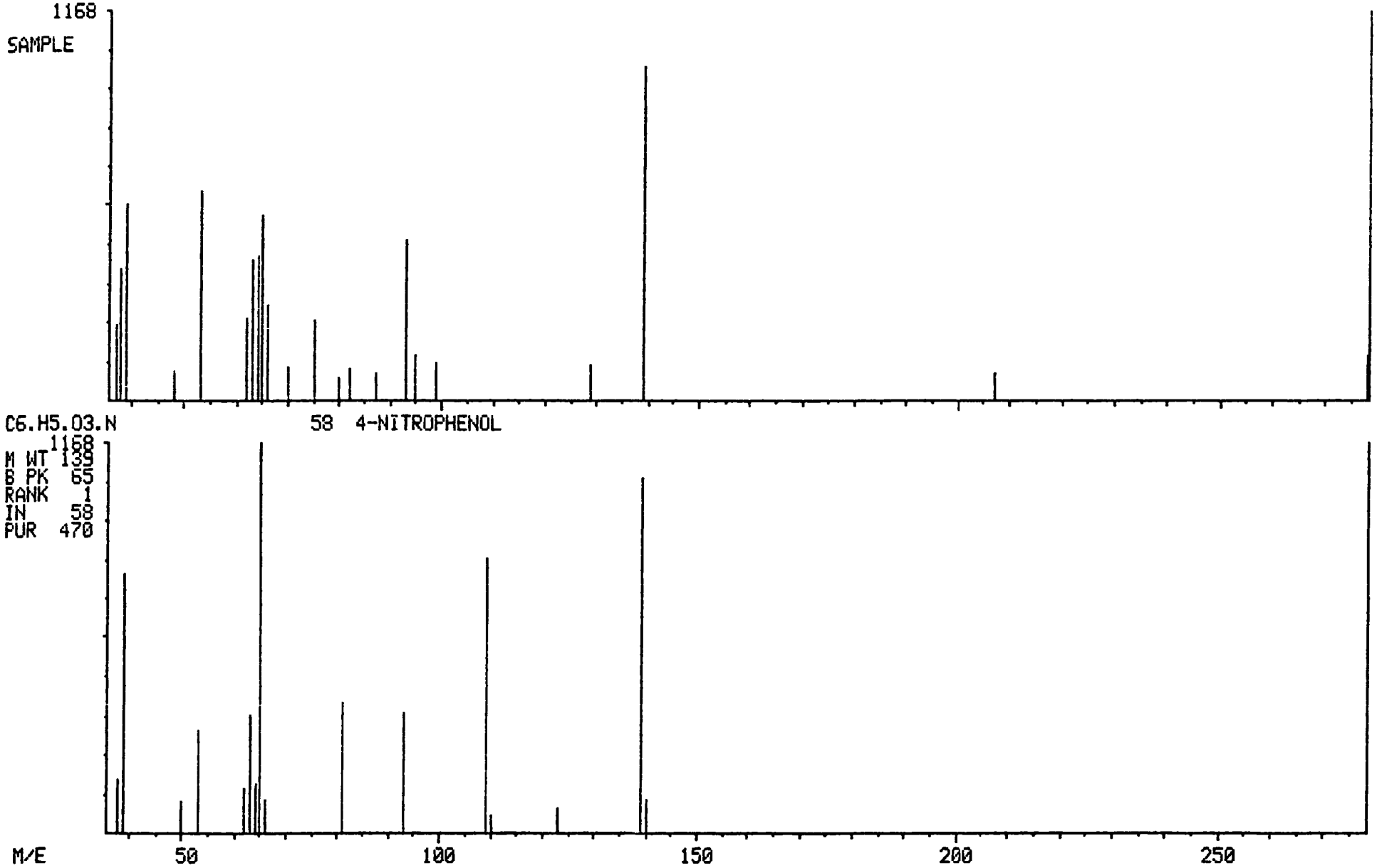
LIBRARY SEARCH
04/28/80 9:55:00 + 8:03
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL
ENHANCED (S 15B 2N 0T)

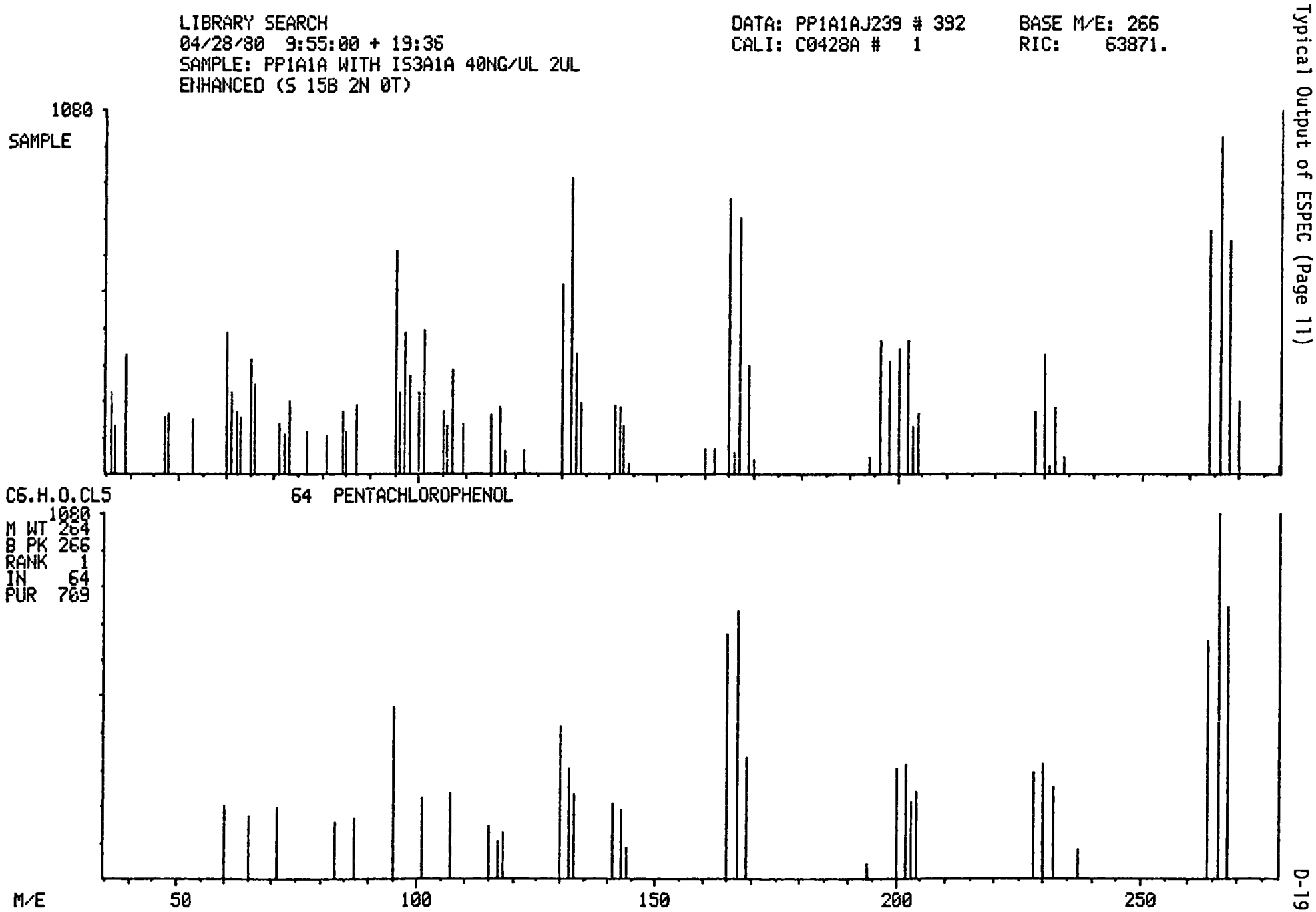
DATA: PP1A1AJ239 # 161 BASE M/E: 139
CALI: C0428A # 1 RIC: 170751.

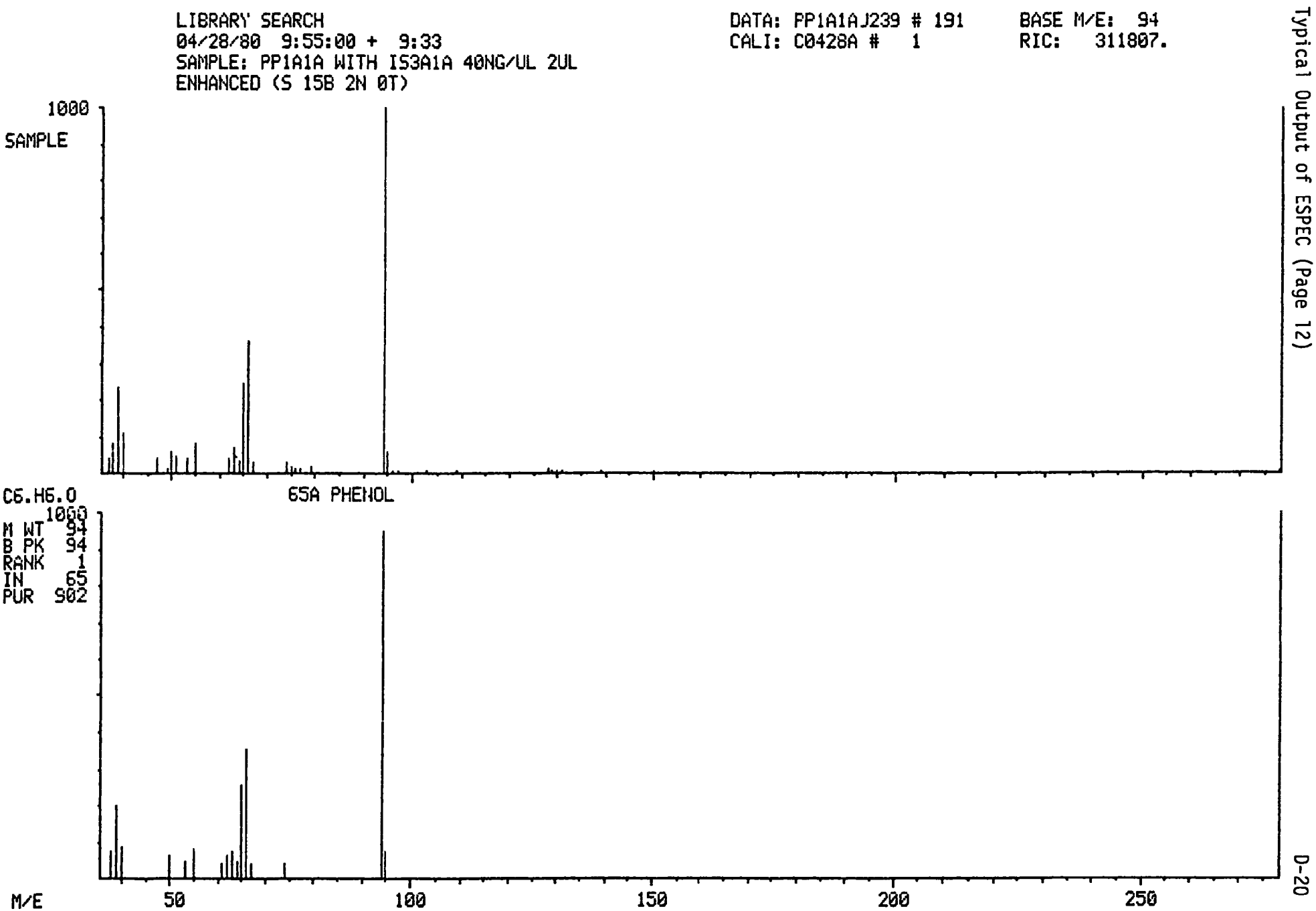


LIBRARY SEARCH
04/28/80 9:55:00 + 27:45
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL
ENHANCED (S 15B 2N 0T)

DATA: PP1A1AJ239 # 555 BASE M/E: 139
CALI: C0428A # 1 RIC: 8127.




LIBRARY SEARCH
04/28/80 9:55:00 + 19:36
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL
ENHANCED (S 15B 2N 0T)
DATA: PP1A1AJ239 # 392
CALI: C0428A # 1
BASE M/E: 266
RIC: 63871.
1080
SAMPLE
C6.H.O.CL5
64 PENTACHLOROPHENOL
1080
M WT 264
B PK 266
RANK 1
IN 64
PUR 769
M/E
50
100
150
200
250



Typical Output of ESPEC (Page 12)

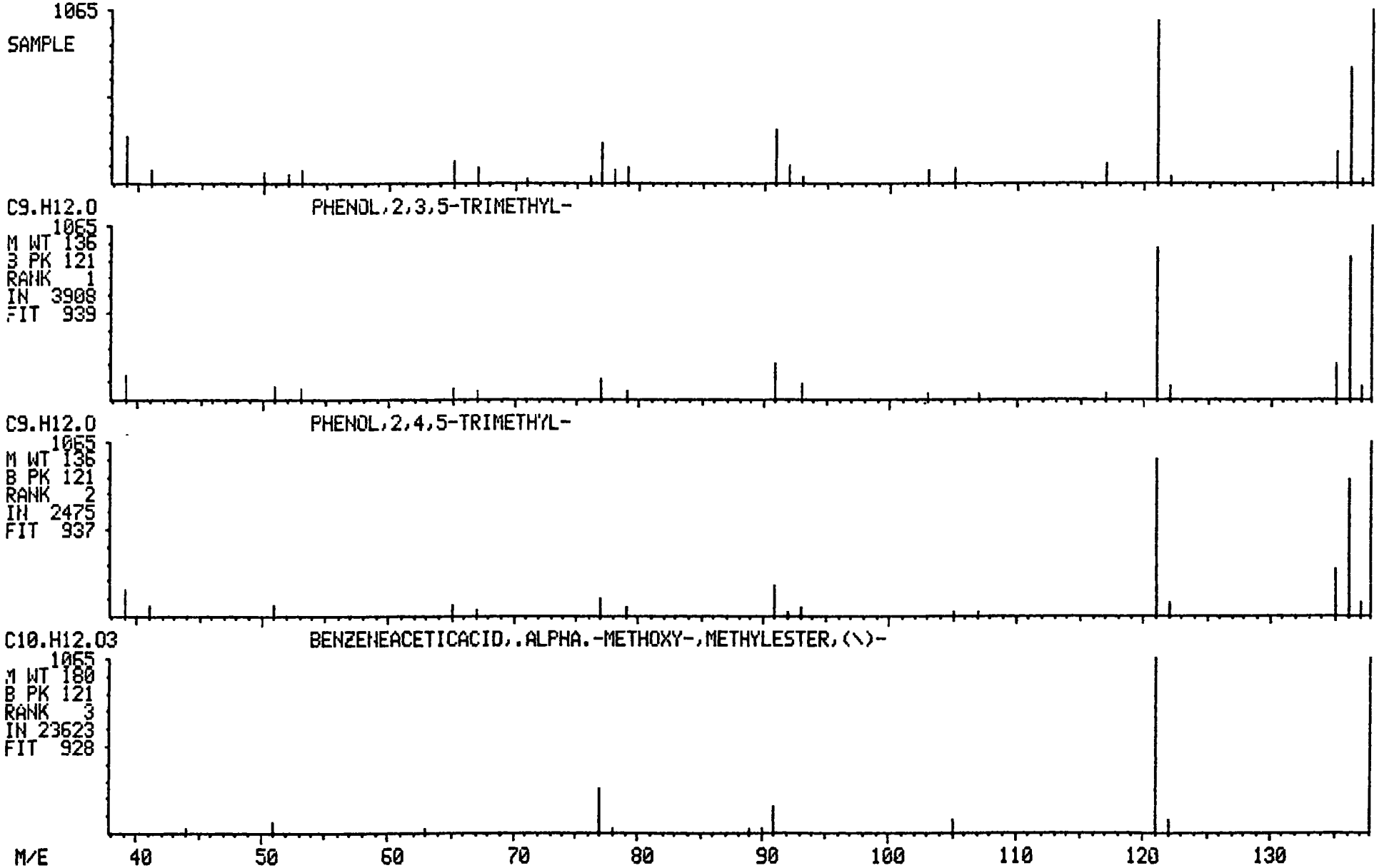
U.S. ENVIRONMENTAL PROTECTION AGENCY
NATIONAL ENFORCEMENT INVESTIGATIONS CENTER
DENVER FEDERAL CENTER BLDG 53 BOX 25227
DENVER, CO 80225

NB LIBRARY SEARCH
FILE: D: PP1A1AJ239.
SPECTRA PRINTOUT AND QUANTITATION REPORT

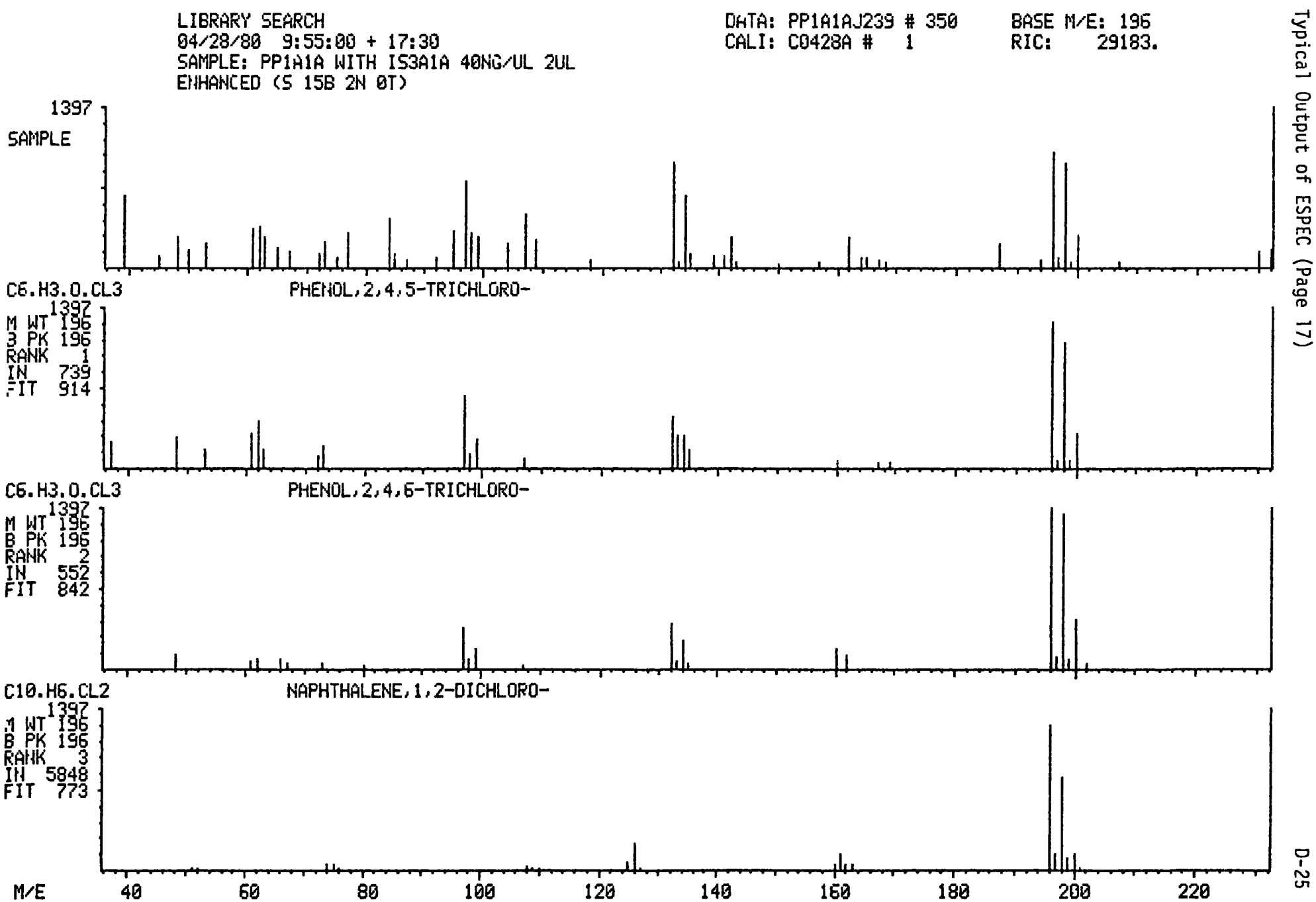
```
LIBRARY SEARCH                DATA:  PP1A1AJ239 #  209    BASE M/E:  121
04/28/80  9:55:00 + 10:27     CALI:  CO 428A  # 1         RIC:       12559.
SAMPLE:  PP1A1A WITH IS3A1A 40NG/UL  2UL
ENHANDED (S 15B 2N OT)

25409 SPECTRA IN LIBRARYNB SEARCHED FOR MAXIMUM FIT
  130 MATCHED AT LEAST 6 OF THE 16 LARGEST PEAKS IN THE UNKNOWN

RANK IN NAME
1  3908 PHENOL,2,3,5-TRIMETHYL-
2  2475 PENOL,2,4,5-TRIMETHYL-
3  23623 BENZENEACETICACIDE, ALPHA -METHOXY-,METHYLESTER,(/)-

RANK FORMULA                              M.WT B.PK   PURITY     FIT    RFIT
1 C9.H12.0                                 136  121     841      939     861
2 C9.H12.0                                 136  121     832      937     849
3 C10.H12.03                               180  121     435      928     457
```

LIBRARY SEARCH
04/28/80 9:55:00 + 10:27
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL
ENHANCED (S 15B 2N 0T)

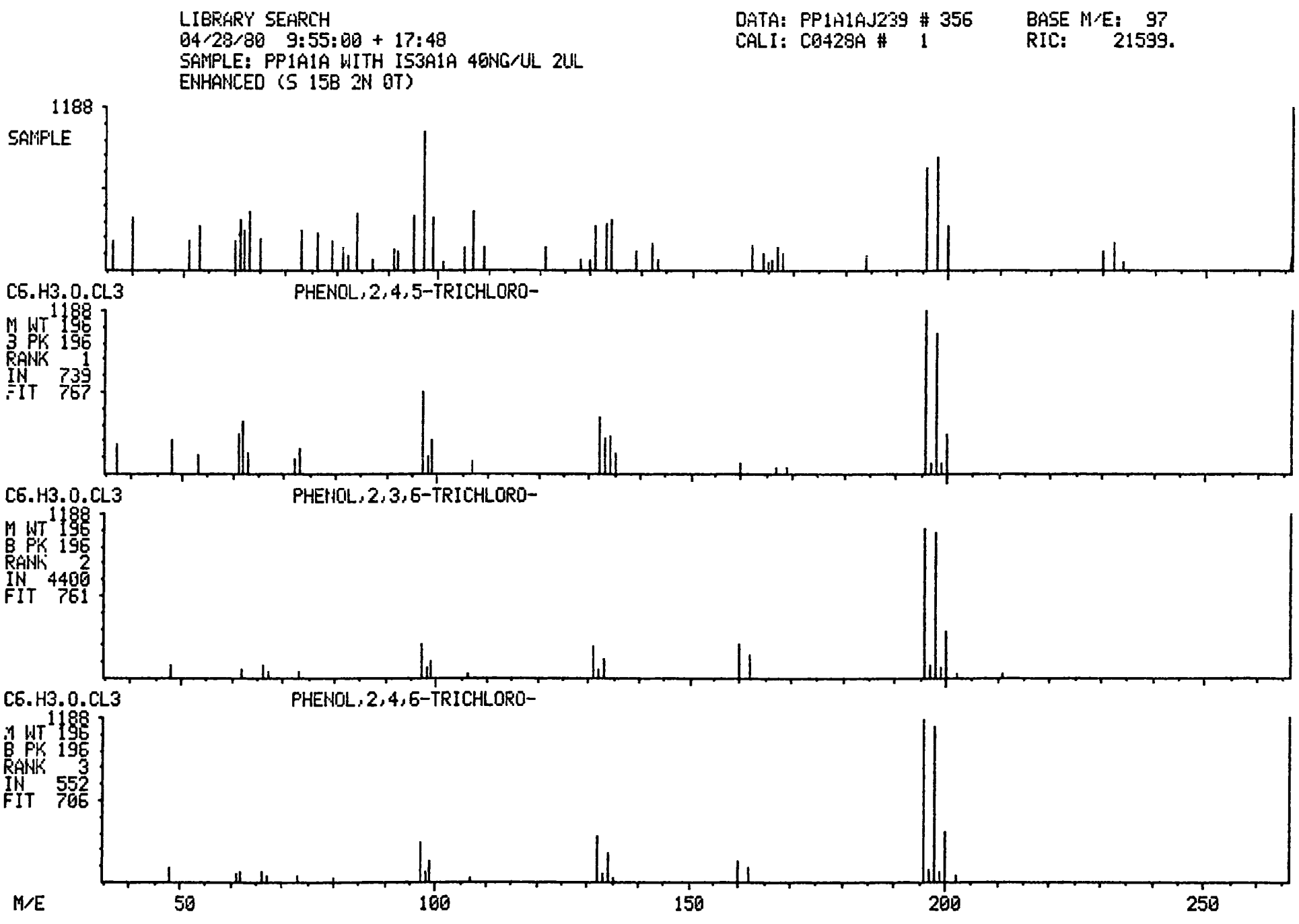
DATA: PP1A1AJ239 # 209 BASE M/E: 121
CALI: C0428A # 1 RIC: 12559.



```
LIBRARY SEARCH                DATA:  PP1A1AJ239 # 350    BASE M/E:     196
04/28/80  9:55:00 + 17:30     CALI:  C0428A #   1        RIC:        29183.
SAMPLE:  PP1A1A WITH IS3A1A 40NG/UL 2UL
ENHANCED (S 15B 2N OT)

25409 SPECTRA IN LIBRARYNB SEARCHED FOR MAXIMUM FIT
  301 MATCHED AT LEAST 3 OF THE 16 LARGEST PEAKS IN THE UNKNOWN

RANK IN NAME
1   739 PHENOL,2,4,5-TRICHLORO-
2   552 PHENOL,2,4,6-TRICHLORO-
3  5848 NAPHTHALENE,1,2-CICHLORO-

RANK FORMULA                        M.WT  B. PK   PURITY   FIT   RFIT
1  C6.H3.O.CL3                       196    196     589     914    608
2  C6.H3.O.CL3                       196    196     545     842    575
3  C10.H6.CL2                        196    196     271     773    324
```


LIBRARY SEARCH
04/28/80 9:55:00 + 17:30
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL
ENHANCED (S 15B 2N 0T)
DATA: PP1A1AJ239 # 350
CALI: C0428A # 1
BASE M/E: 196
RIC: 29183.
1397
SAMPLE
C6.H3.O.CL3
PHENOL,2,4,5-TRICHLORO-
1397
M WT 196
B PK 196
RANK 1
IN 739
FIT 914
C6.H3.O.CL3
PHENOL,2,4,6-TRICHLORO-
1397
M WT 196
B PK 196
RANK 2
IN 552
FIT 842
C10.H6.CL2
NAPHTHALENE,1,2-DICHLORO-
1397
M WT 196
B PK 196
RANK 3
IN 5848
FIT 773
M/E
40
60
80
100
120
140
160
180
200
220

```
LIBRARY SEARCH                DATA:  PP1A1AJ239 # 356    BASE M/E:     97
04/28/80  9:55:00 + 17:48     CALI:  C0428A #   1        RIC:       21599.
SAMPLE:  PP1A1A WITH IS3A1A 40NG/UL 2UL
ENHANCED (S 15B 2N OT)

25409 SPECTRA IN LIBRARYNB SEARCHED FOR MAXIMUM FIT
  266 MATCHED AT LEAST 3 OF THE 16 LARGEST PEAKS IN THE UNKNOWN

RANK FORMULA
1   739 PHENOL,2,4,5-TRICHLORO-
2  4400 PHENOL,2,3,6-TRICHLORO-
3   552 PHENOL,2,4,6-TRICHLORO-

RANK FORMULA                      M.WT  B. PK   PURITY   FIT   RFIT
1  C6.H3.O.CL3                    196    196     421     767    515
2  C6.H3.O.CL3                    196    196     355     761    425
3  C6.H3.CL3                      196    196     367     706    447
```


LIBRARY SEARCH
04/28/80 9:55:00 + 17:48
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL
ENHANCED (S 15B 2N 0T)
DATA: PP1A1AJ239 # 356
CALI: C0428A # 1
BASE M/E: 97
RIC: 21539.
1188
SAMPLE
C6.H3.O.CL3
PHENOL,2,4,5-TRICHLORO-
1188
M WT 196
B PK 196
RANK 1
IN 739
FIT 767
C6.H3.O.CL3
PHENOL,2,3,6-TRICHLORO-
1188
M WT 196
B PK 196
RANK 2
IN 4400
FIT 761
C6.H3.O.CL3
PHENOL,2,4,6-TRICHLORO-
1188
M WT 196
B PK 196
RANK 3
IN 552
FIT 706
M/E
50
100
150
200
250

U.S. ENVIRONMENTAL PROTECTION AGENCY
NATIONAL ENFORCEMENT INVESTIGATIONS CENTER
DENVER FEDERAL CENTER BLDG 53 BOX 25227
DENVER, CO 80225

QUANTITATION REPORT FILE: EVAL

DATA: PP1A1AJ239.TI
04/28/80 9:55:00
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL
CONDS.: 70-190 8C/MIN
FORMULA: INSTRUMENT: 3200EI WEIGHT: 0.000
SUBMITTED BY: JFC ANALYST: JFC ACCT. NO.: J239

AMOUNT=AREA * REF.AMNT/(REF.AREA* RESP.FACT)

NO	NAME
1	ISA D10-PHENANTHRENE (133)
2	PHENOL,2,3,5-TRIMETHYL-
3	PHENOL,2,3,5-TRIMETHYL-
4	PHENOL,2,4,5-TRICHLORO-
5	PHENOL,2,4,5-TRICHLORO-

NO	M/E	SCAN	TIME	REF	RRT	METH	AREA	AMOUNT	%TOT
1	188	343	17:09	1	1.000	A BB	336606.	40.000 NG/UL	57.16
2	TOT	205	10:15	1	0.598	A BB	66.8.	0.786	1.12
3	TOT	209	10.27	1	0.609	A BB	31724.	3.770	5.39
4	TOT	350	17:30	1	1.020	A BV	95456.	11.343	16.21
5	TOT	356	17:48	1	1.038	A VB	118487.	14.080	20.12

APPENDIX E

Operation of Procedure ISCHK

Procedure ISCHK

Typical Output of ISCHK

> ISCHK FILENAME, , LIBRARY LIST is the command that initiates the procedure.

This procedure locates and quantitates the internal standard(s) in standard mixture runs and in sample runs. The procedure is driven by a library list. The library lists used with ISCHK currently are ACCHK for acids, BNCHK for base/neutrals, VOLCHK for volatiles in water, and AIRCHK for volatiles in air.

Create Library Lists containing the compound name(s) of the internal standard(s) listed in each standard mixture library list. The internal standard used for quantitation must be the first entry in the library list.

```
>EDLL ACCHK
(Store library list name.)
EDLL: $PP, 133
(Append entry #133 from Library PP to list.)
```

Load all entries.

```
EDLL: W;E
```

ISCHK generates a copy of instrument parameters at the time of the GC/MS run, a mass chromatogram for each internal standard, an RIC, a quantitation list, and a quantitation report. Check the peak shape of the mass chromatogram for any abnormalities such as splitting of the peak. An internal standard cannot be used for quantitation or relative retention time calculation if the peak is split. Record the peak area of the internal standard(s). Calculate the experimental limits of the IS peak area at its standard concentration. If the IS area of a run exceeds the experimental limits established by the operator, the standard run or sample run must be rejected.

```
TRACE OF PROCEDURE ISCHK
   * ERASE
   * ;[ PROCEDURE ISCHK                                                    ]
   * ;[ >ISCHK FILENAME,,LIBRARY LIST  EXECUTES THE PROCEDURE.            ]
   * ;[                                                                    ]
   * ;[ WRITTEN BY BA HUGHES  MARCH,1980  LAST REVISION 03/20/80 BAH       ]
   * ;[                                                                    ]
   * ;[ THIS PROCEDURE LOCATES AND QUANTITATES THE INTERNAL STANDARD       ]
   * ;[ COMPOUND(S) STORED IN THE LIBRARY LIST. ISCHK USES INFORMATION     ]
   * ;[ FROM AND STORES INFORMATION ON DISK DRIVE UNIT#0.                  ]
   * ;PARA (I;H;E)
   * ;SETQ CHK
   * ;EDQL CHK (-;W;E)
   * ;SETL $3#0
   * ;ISCHK1
   * ;CHRO (H1,2000;E)
   * ;EDQL CHK (I;H;E)
   * ;QUAN CHK (I;F2;H;E)
   * ;FEED;BEEP
   * ;[ PROCEDURE ISCHK IS COMPLETE.  ]
   *
   ERASE
   PARA  (I;H;E)
   SETQ CHK
   EDQL CHK (-;W;E)
   SETL $3
   ISCHK1
      * ;GETL
      * ;CHRO (I;R;$;&;#;N1,2;A>5,3;G-4,4;D-10,10;H-10,10;E)
      * ;LOOP
      *
      GETL
      CHRO  (I;R;$;&;#;N1,2;A>5,3;G-4,4;D-10,10;H-10,10;E)
      LOOP
   CHRO  (H1,2000;E)
   EDQL CHK (I;H;E)
   QUAN CHK (I;F2;H;E)
   FEED
   BEEP
```

```
INPUT FILE: ACCHK.LL, OUTPUT FILE. ACCHK.LL
PP,    133   PP,    135
```

NAM	NUM:	WT	FORMULA	NAME
PP	133:	188	C14.D10	ISA D10-PHENANTHRENE (133)
PP	135:	136	C8.D8	ISA D8-NAPHTHALENE (135)

INPUT FILE: BNCHK.LL, OUTPUT FILE: BNCHK.LL
PP, 129 PP, 136

NAM	NUM:	WT	FORMULA	NAME
PP	129:	212	C16.D10	ISB D10-PYRENE (129)
PP	136:	136	C8.D8	ISB D8-NAPHTHALENE (136)

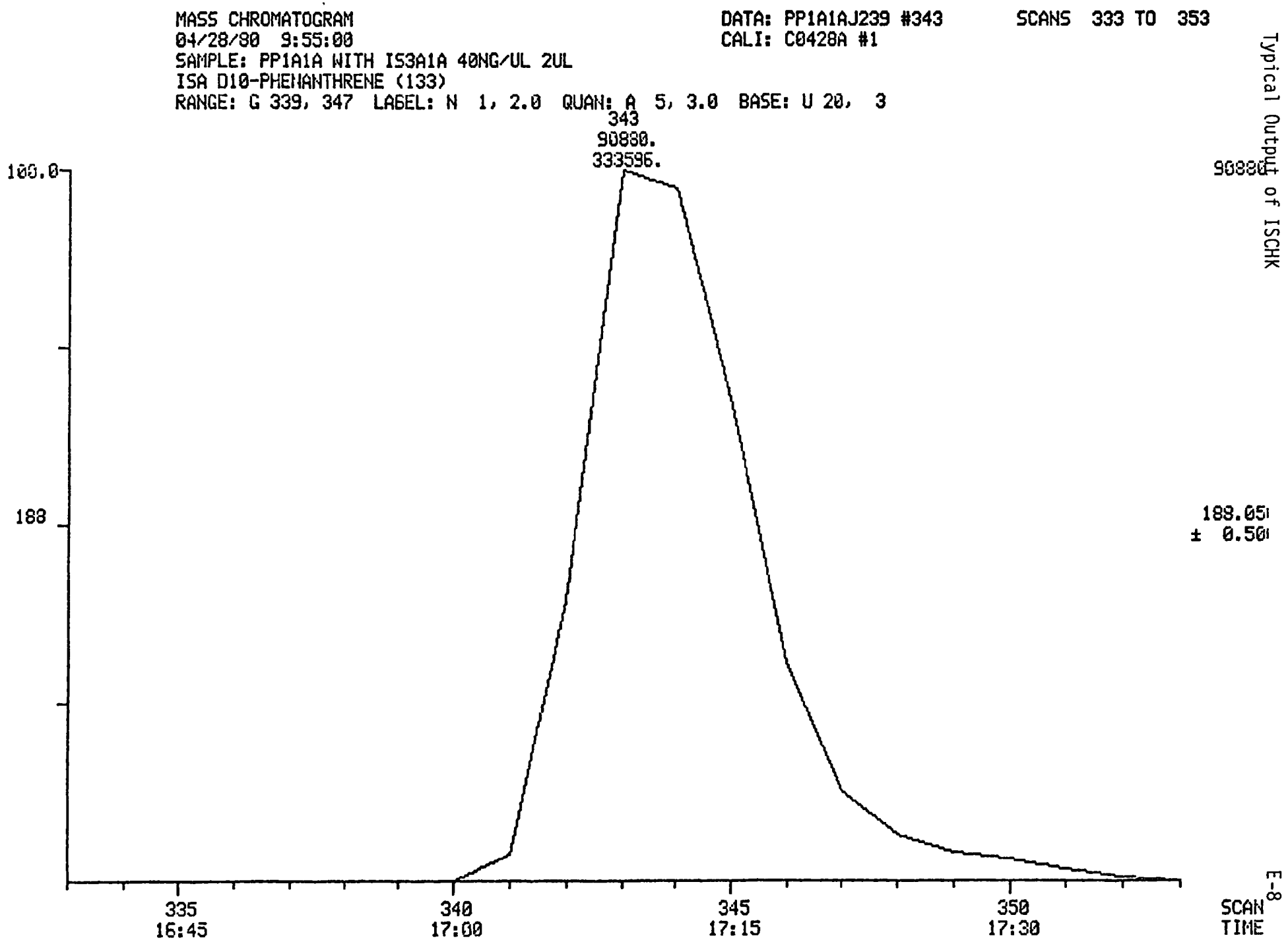
INPUT FILE: VOLCHK.LL, OUTPUT FILE: VOLCHK.LL
PP, 122 PP, 123

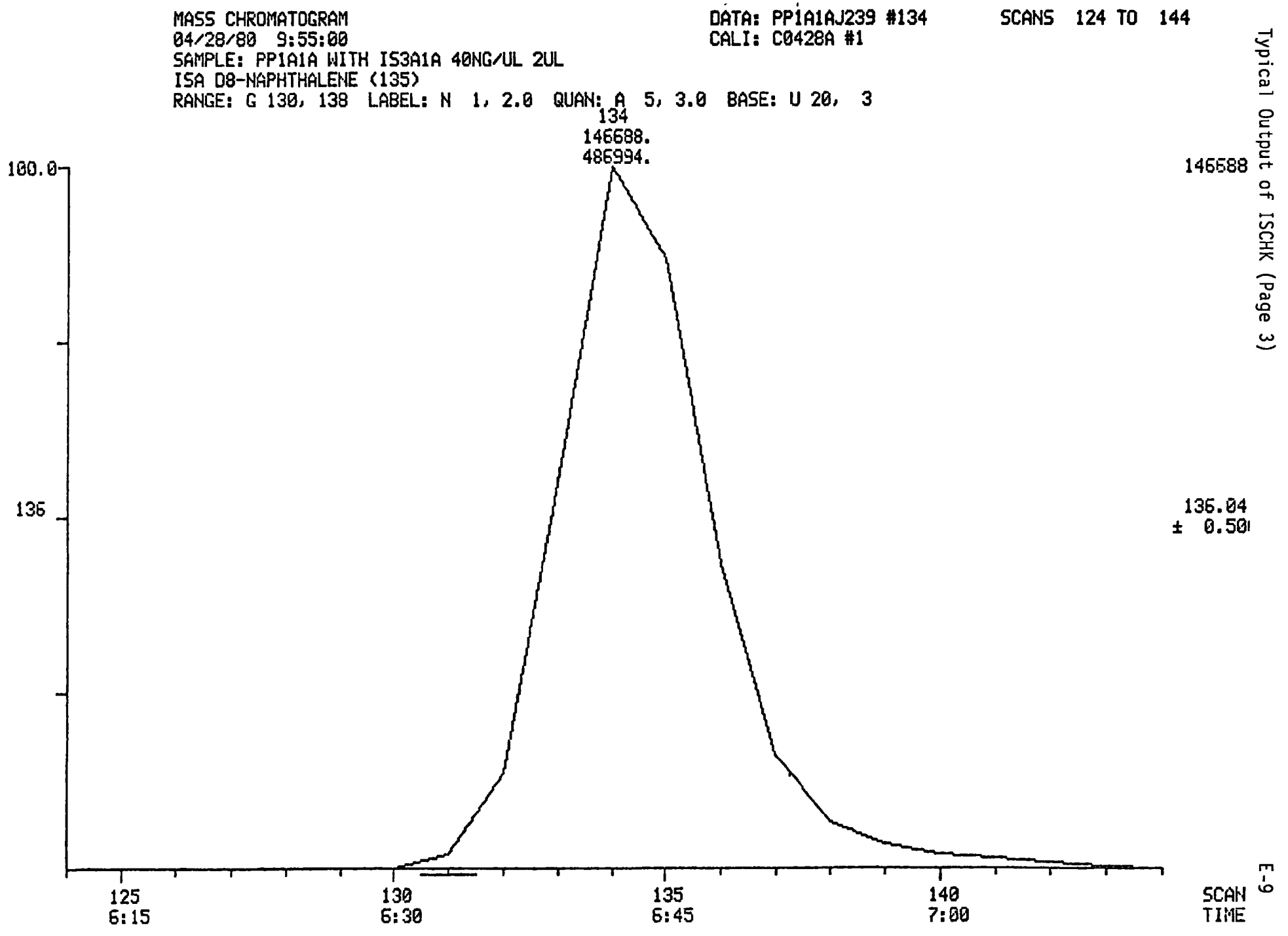
NAM	NUM:	WT	FORMULA	NAME
PP	122:	126	C4. H8. CL2	ISV 1,4-DICHLOROBUTANE (122)
PP	123:	128	C. H2. CL. BR	ISV BROMOCHLOROMETHANE (123)

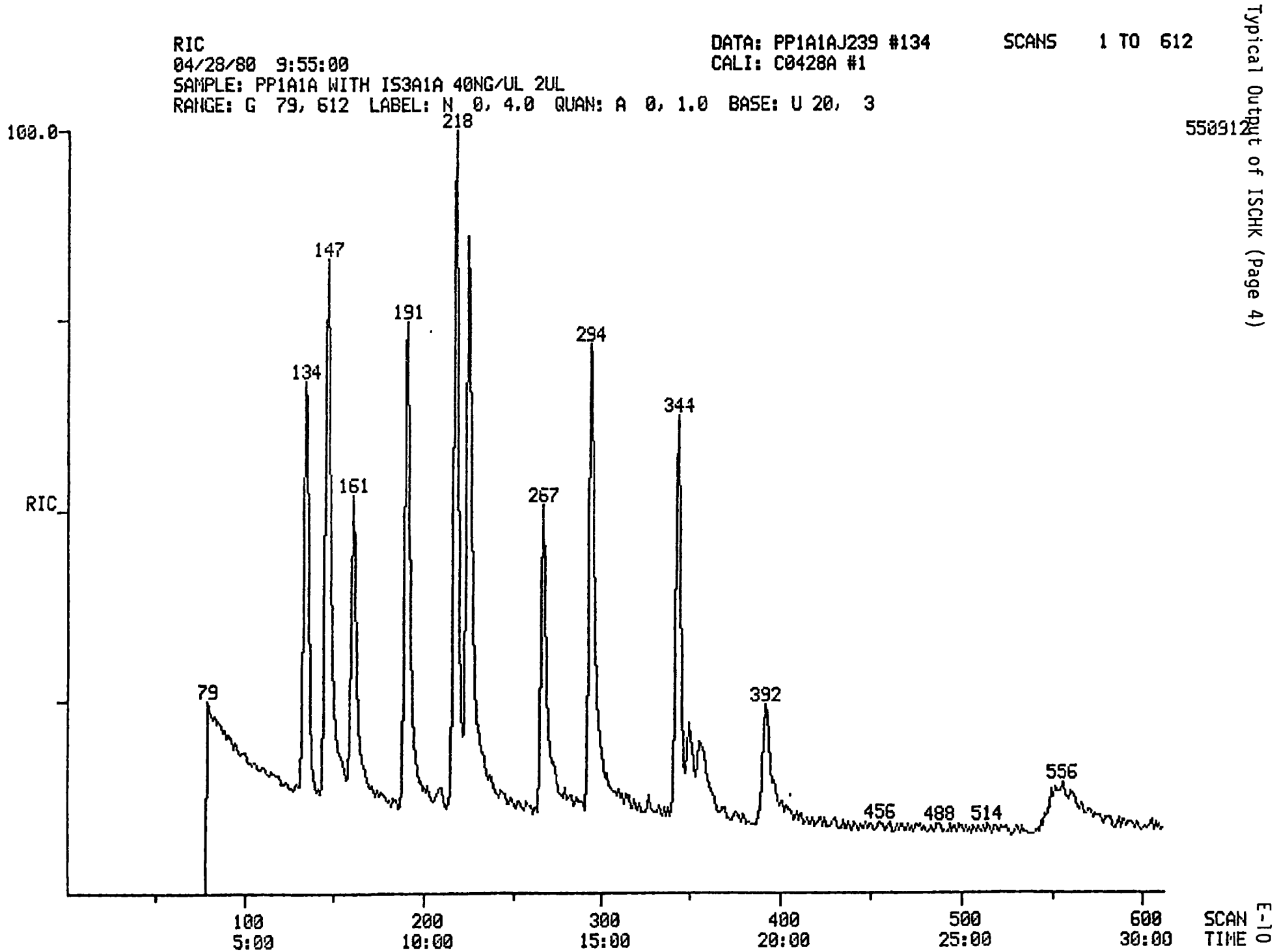
INPUT FILE: AIRCHK.LL, OUTPUT FILE: AIRCHK.LL
PP, 125

NAM NUM:	WT	FORMULA	NAME
PP 125:	186	C6.F6	AIS HEXAFLUOROBENZENE (125)

```
PARAMETERS                          DATA: PP1A1AJ239 TI (PP1A1AJ239 MI)
04/28/80  9 55 00 + 30 36           CALI  C0428A              SCANS   79 TO  612
SAMPLE  PP1A1A WITH IS3A1A 40NG/UL 2UL
CONDS   70-190 8C/MIN
FORMULA                             INSTRUMENT  3200EI        WEIGHT:     0.000
SUBMITTED BY: JFC                   ANALYST. JFC              ACCT. NO    J239

ACC. VOL      8000                  THRESHOLD         2       INTEN/ION         2
A/D S.I .    0 025                  CENT S.I .    0 200       FRAG S I      1 200
PEAK WIDTH:   1000                  CENT SAMP/PK     56       FRAG SAMP/PK:     9
MIN  WIDTH       2                  MIN  FRAG  WIDTH (%)  80  MIN AREA         75

612 SCANS (355 SECTORS) OF LINEAR UP CENTROID DATA

LOW MASS:     35  SCAN TIMES (SECS ) UP:   2 95       TOP.   0 00
HIGH MASS    300                     DOWN:  0 00    BOTTOM   0 05

THERE IS A SCAN LIST WITH     0 ENTRIES

THERE IS A QUANTITATION LIST WITH  13 ENTRIES
```


MASS CHROMATOGRAM
04/28/80 9:55:00
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL
ISA D10-PHENANTHRENE (133)
RANGE: G 339, 347 LABEL: N 1, 2.0 QUAN: A 5, 3.0 BASE: U 20, 3
DATA: PP1A1AJ239 #343
CALI: C0428A #1
SCANS 333 TO 353
343
90880.
333596.
100.0
188
90880
188.05
± 0.50
E-8
335
16:45
340
17:00
345
17:15
350
17:30
SCAN
TIME
Typical Output of ISCHK


MASS CHROMATOGRAM
04/28/80 9:55:00
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL
ISA D8-NAPHTHALENE (135)
RANGE: G 130, 138 LABEL: N 1, 2.0 QUAN: A 5, 3.0 BASE: U 20, 3
DATA: PP1A1AJ239 #134
CALI: C0428A #1
SCANS 124 TO 144
134
146688.
486994.
100.0
146588
136
136.04
± 0.50
125
6:15
130
6:30
135
6:45
140
7:00
SCAN
TIME
Typical Output of ISCHK (Page 3)
E-9


RIC
04/28/80 9:55:00
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL
RANGE: G 79, 612 LABEL: N 0, 4.0 QUAN: A 0, 1.0 BASE: U 20, 3
DATA: PP1A1AJ239 #134
CALI: C0428A #1
SCANS 1 TO 612
550912
100.0
RIC
218
147
191
134
294
344
161
267
79
392
556
456
488
514
100
5:00
200
10:00
300
15:00
400
20:00
500
25:00
600
30:00
SCAN
TIME
Typical Output of ISCHK (Page 4)

INPUT FILE: CHK.QL, OUTPUT FILE: CHK.QL

REFERENCE RETENTION TIME (MIN:SEC) 6:42

NO.	LOW MASS	HIGH	SCAN	TIME	METH	AREA	HEIGHT	NAME	NUM
1	187.56	188.56	343	17:09	A BB	333596.	90880.	PP	133
2	135.54	136.54	134	6:42	A BB	486994.	146688.	PP	135

QUANTITATION REPORT FILE: CHK

DATA: PP1A1AJ239.TI
04/28/80 9:55:00
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL
CONDS.: 70-190 8C/MIN
FORMULA: INSTRUMENT: 3200EI WEIGHT: 0.000
SUBMITTED BY: JFC ANALYST: JFC ACCT. NO.: J239

AMOUNT=AREA * REF.AMNT/(REF.AREA* RESP.FACT)

NO	NAME
1	ISA D10-PHENANTHRENE (133)
2	ISA D8-NAPHTHALENE (135)

NO	M/E	SCAN	TIME	REF	RRT	METH	AREA	AMOUNT	%TOT
1	188	343	17:09	1	1.000	A BB	333596.	40.000 NG/UL	49.78
2	136	134	6:42	1	0.391	A BB	486994.	40.361 NG/UL	50.22

NO	RET(L)	RATIO	RRT(L)	RATIO	AMNT	AMNT(L)	R.FAC	R.FAC(L)	RATIO
1	17:09	1.00	1.000	1.00	40.00	40.00	1.000	1.000	1.00
2	6:42	1.00	0.391	1.00	40.36	40.00	1.460	1.447	1.01

APPENDIX F

Operation of MQIS

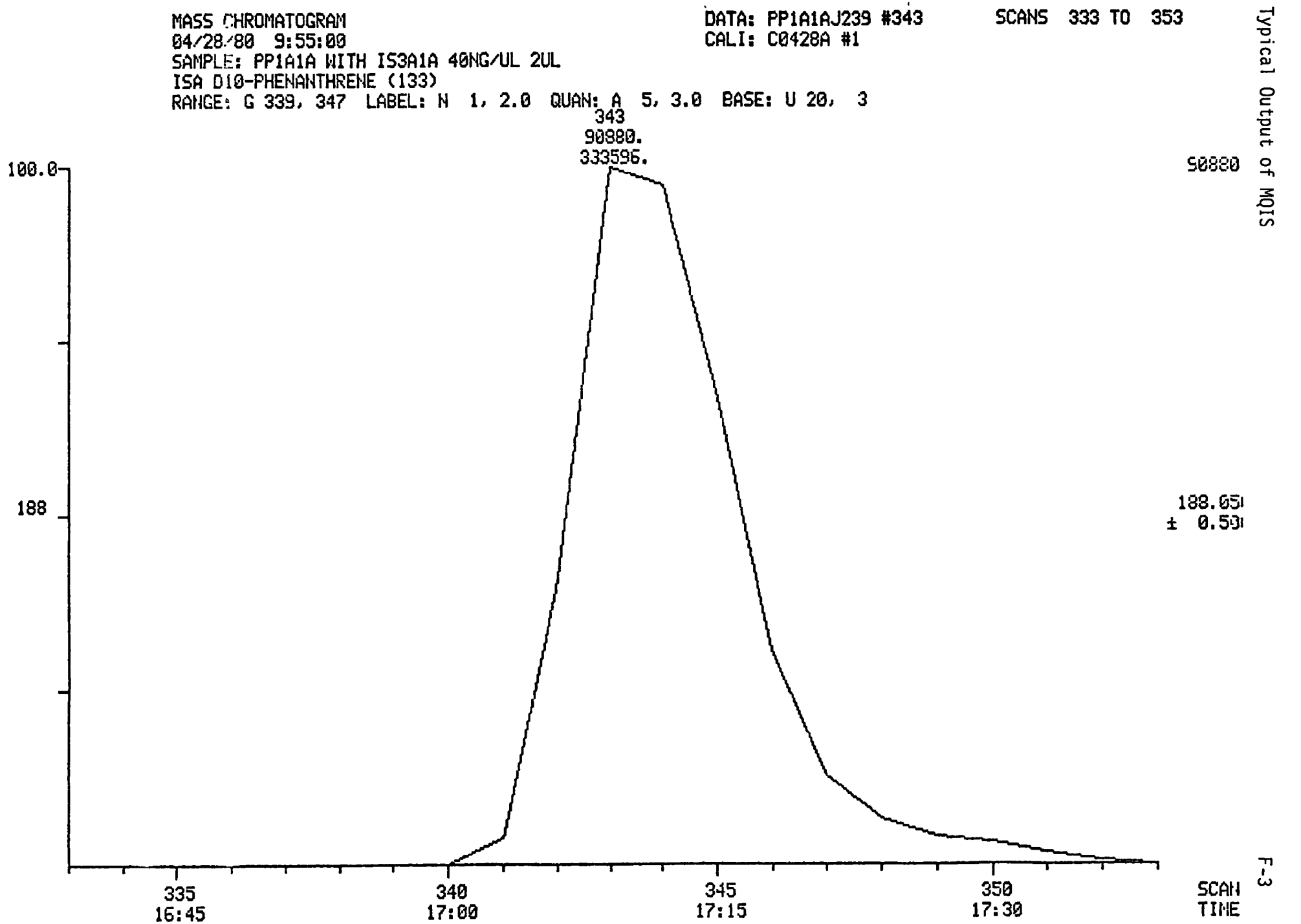
Procedure MQIS

Typical Output of MQIS

>MQIS FILENAME#SCAN, LIBRARY NAME, #LIBRARY ENTRY is the command that initiates the procedure.

This procedure locates and quantitates an internal standard peak in a standard mixture run using the scan number and priority pollutant number read in the execution statement. The quantitation results are appended to CHK.QL. MQIS is used when ISCHK fails to locate the internal standard(s).

```
TRACE OF PROCEDURE MQIS
   * ERASE
   * ;[ PROCEDURE MQIS                                                    ]
   * ;[ >MQIS   FILENAME#SCAN,LIBRARY NAME,#LIBRARY ENTRY  EXECUTES      ]
   * ;[ THE PROCEDURE.                                                    ]
   * ;[                                                                   ]
   * ;[ WRITTEN BY BA HUGHES  MARCH,1980  LAST REVISION 03/21/80 BAH      ]
   * ;[                                                                   ]
   * ;[ MQIS IS A PROCEDURE THAT LOCATES AND QUANTITATES AN INTERNAL      ]
   * ;[ STANDARD PEAK USING THE SCAN# AND PP# READ IN THE EXECUTION       ]
   * ;[ STATEMENT.  THE QUANTITATION RESULTS ARE APPENDED TO QUAN FILE    ]
   * ;[ CHK.  MQIS IS USED WHEN ISCHK FAILS TO LOCATE THE INTERNAL        ]
   * ;[ STANDARD(S).                                                      ]
   * ;SET4 $2
   * ;SET4 #!3
   * ;SETQ CHK
   * ;CHRD(I;R;$;#;N1,2;A>5,3;G-4,4;D-10,10;H-10,10;E)
   * ;FEED;BEEP
   *
   ERASE
   SET4 $2
   SET4 !3
   SETQ CHK
   CHRD  (I;R;$;#;N1,2;A>5,3;G-4,4;D-10,10;H-10,10;E)
   FEED
   BEEP
```


MASS CHROMATOGRAM
04/28/80 9:55:00
SAMPLE: PP1A1A WITH IS3A1A 40NG/UL 2UL
ISA D10-PHENANTHRENE (133)
RANGE: G 339, 347 LABEL: N 1, 2.0 QUAN: A 5, 3.0 BASE: U 20, 3
DATA: PP1A1AJ239 #343
CALI: C0428A #1
SCANS 333 TO 353
343
90880.
333596.
100.0
188
90880
188.05
± 0.59
335
16:45
340
17:00
345
17:15
350
17:30
SCAN
TIME
Typical Output of MQIS
F-3

APPENDIX G

Operation of ESETØ

Procedure ESETØ

>ESETØ FILENAME, CALIBRATION FILE, LIBRARY LIST activates the procedure.

This procedure allows one to locate and quantitate standard compound peaks in a standard mixture run using the scan numbers read from a scan list and the priority pollutant numbers read from a library list. The priority pollutant numbers link the names of the standard compounds identified manually in the chromatographic run to the names of the standard compounds in the Priority Pollutant Library (Master User Library). The quantitation results are appended to a quantitation list having the same name as the Filename. The library list should be in order of increasing priority pollutant number with the internal standard(s) as the first entry. The scan list must follow the order dictated by the library list.

Compound Name	Library List Entry	Scan #
d10-Phenanthrene (IS)	PP 133	343
d8-Naphthalene (IS)	PP 135	134
2,4,6-Trichlorophenol	PP 21	267
4-Chloro-3-methylphenol	PP 22	294
2-Chlorophenol	PP 24	147
2,4-Dichlorophenol	PP 31	225
2,4-Dimethylphenol	pp 34	218

Create a library list or use an existing standard mixture library list. The library lists currently being used are PPPH.LL for acids, PPBN.LL for base/neutrals, PPVOL.LL for volatiles in water and PPAIR.LL for volatiles in air.

```
>EDLL NAME
EDLL: $PP, 133; 135; 21; 22; 24; 31; 34
EDLL: W;E
```

Create a scan list where each scan number corresponds to each library list entry.

```
>EDSL FILENAME
EDSL: 343; 134; 267; 294; 147; 225; 218
EDSL: W;E
```

ESETØ generates a quantitation list. Edit the QUAN list to update the standard compound response factors(R), relative retention times (S), and retention times (T) in the Priority Pollutant Library. ESETØ is most useful when the chromatographic conditions for a standard mixture have been changed but the component members and standard amount have remained the same.

```
TRACE OF PROCEDURE ESETO
   * ERASE
   * ;[ PROCEDURE ESETO - 12/11/79 BAH   MODIFIED 01/08/80 DJL          ]
   * ;[ FORMERLY EVALUP                                                 ]
   * ;[ THIS PROCEDURE ALLOWS ONE TO UPDATE RESPONSE FACTORS (R),       ]
   * ;[ RELATIVE RETENTION TIMES (S), RETENTION TIMES (T) IN USER       ]
   * ;[ LIBRARIES. THE PROCEDURE IS MOST USEFUL WHEN NO OTHER           ]
   * ;[ PARAMETERS ARE TO BE CHANGED. BEFORE EXECUTING THIS PROGRAM,    ]
   * ;[ CREATE A LIBRARY LIST AND A SCAN LIST (FILENAME.SL) FOR THE     ]
   * ;[ STANDARD MIX. THE .LL SHOULD BE IN ORDER OF INCREASING          ]
   * ;[ PRIORITY POLLUTANT NUMBER AND THE .SL MUST FOLLOW THE ORDER     ]
   * ;[ DICTATED BY THE LIBRARY LIST. EDIT THE QUAN LIST GENERATED      ]
   * ;[ BY EVALUP TO UPDATE R,S,T.                                      ]
   * ;[                                                                 ]
   * ;[ ******** USE THIS PROCEDURE FOR FILES ON UNIT 0: *******        ]
   * ;[ >ESETO  FILENAME,CALIBRATION FILE, LIBRARY LIST                 ]
   * ;[ ACTIVATES THE PROCEDURE.                                        ]
   * ;[                                                                 ]
   * ;SETL $3#0
   * ;SETQ $1
   * ;EDQL(-;W;E)
   * ;SETS $1#0
   * ;ESETA
   * ;BEEP;BEEP;BEEP
   * ;ERASE
   * ;[ PROCEDURE ESETO IS DONE ]
   *
   ERASE
   SETL $3
   SETQ $1
   EDQL  (-;W;E)
   SETS $1
   ESETA
      * ;[ PART OF ESETO (FORMERLY EVALUP)]
      * ;GETL
      * ;GETS
      * ;CHRO(I;R;$;#;N1,2;A>5,3;G-4,4;D-10,10;E)
      * ;LOOP
      *
      GETL
      GETS
      CHRO  (I;R;$;#;N1,2;A>5,3;G-4,4;D-10,10;E)
      LOOP
   BEEP
   BEEP
   BEEP
   ERASE
```

APPENDIX H

Operation of ESET2

Procedure ESET2

>ESET2 FILENAME, CALIBRATION FILE, LIBRARY LIST activates the procedure.

This procedure is similar in operation to ESETØ. The procedure is used to process data files stored on Unit #2 of a Two-Disk-Drive System. The library list must be stored on Unit #3.

```
>EDLL 3: NAME
EDLL: $PP, 133; 135, 21; 22; 24; 31; 34
EDLL: W;E
```

Store the scan list on Unit #2.

```
>EDSL 2: FILENAME
EDSL: 343; 134; 267; 294; 147; 225; 218
EDSL: w;E
```

The quantitation results are appended to a quantitation list stored on Unit #2. To edit or examine the quantitation list,

```
>EDQL 2:Filename
```

```
TRACE OF PROCEDURE ESET2
   * ERASE
   * ;[ PROCEDURE ESET2  - 12/11/79 BAH    MODIFIED 01/08/80 OJL        ]
   * ;[ FORMERLY EVALUP                                                 ]
   * ;[ THIS PROCEDURE ALLOWS ONE TO UPDATE RESPONSE FACTORS (R),       ]
   * ;[ RELATIVE RETENTION TIMES (S), RETENTION TIMES (T) IN USER       ]
   * ;[ LIBRARIES. THE PROCEDURE IS MOST USEFUL WHEN NO OTHER           ]
   * ;[ PARAMETERS ARE TO BE CHANGED. BEFORE EXECUTING THIS PROGRAM,    ]
   * ;[ CREATE A LIBRARY LIST AND A SCAN LIST (FILENAME.SL) FOR THE     ]
   * ;[ STANDARD MIX. THE .LL SHOULD BE IN ORDER OF INCREASING          ]
   * ;[ PRIORITY POLLUTANT NUMBER AND THE .SL MUST FOLLOW THE ORDER     ]
   * ;[ DICTATED BY THE LIBRARY LIST. EDIT THE QUAN LIST GENERATED      ]
   * ;[ BY EVALUP TO UPDATE R,S,T.                                      ]
   * ;[                                                                 ]
   * ;[   ****** USE THIS PROCEDURE FOR FILES ON UNIT 2:               ]
   * ;[   ****** THE LIBRARY LIST MUST BE COPIED ONTO UNIT 3: ******   ]
   * ;[                                                                 ]
   * ;[ >ESET2  FILENAME,CALIBRATION FILE, LIBRARY LIST                 ]
   * ;[ ACTIVATES THE PROCEDURE.                                        ]
   * ;[                                                                 ]
   * ;SETL 3:$3#0
   * ;SETQ 2:$1
   * ;EDQL(-;W;E)
   * ;SETS 2:$1#0
   * ;ESETA
   * ;BEEP;BEEP;BEEP
   * ;ERASE
   * ;[ PROCEDURE ESET2 IS DONE ]
   *
   ERASE
   SETL 3:$3
   SETQ 2:$1
   EDQL  (-;W;E)
   SETS 2:$1
   ESETA
      * ;[ PART OF ESETO (FORMERLY EVALUP)]
      * ;GETL
      * ;GETS
      * ;CHRO(I;R;$;#;N1,2;A>5,3;G-4,4;D-10,10;E)
      * ;LOOP
      *
      GETL
      GETS
      CHRO  (I;R;$;#;N1,2;A>5,3;G-4,4;D-10,10;E)
      LOOP
   BEEP
   BEEP
   BEEP
   ERASE
```

APPENDIX I

Operation of EVALØQ

Procedure EVALØQ

>EVALØQ FILENAME, LIBRARY LIST initiates the procedure.

This procedure locates standard compound peaks in a standard mixture run using a fixed relative retention time window calculated in the procedure and based on the relative retention time for each compound stored in the Priority Pollutant Library. The procedure quantitates the standard peaks using the ion used for quantitation and the response factor for each compound stored in the Priority Pollutant Library. EVALØQ is driven by a library list containing the component names in a standard compound mixture, such as PPPH.LL for acids. EVALØQ generates a quantitation list and a quantitation report listing all of the compounds in the library list.

EVALØQ is a shortened version of EVALØ. It is used to evaluate daily standard runs and update the retention times, relative retention times, and response factors for each compound. Updating these parameters permits a correction for small daily variation in instrument response. EVALØQ is used mainly for rapid processing of the daily standard before batch processing of sample data.

```
TRACE OF PROCEDURE EVALOQ
   * ERASE
   * ,[ PROCEDURE EVALØQ                                          ]
   * ,[ WRITTEN BY OJLOGSDON 1/8/80                               ]
   * ,[ BASED ON THE ORIGINAL EVALQ BY DHUGHES                     ]
   * ,[                                                           ]
   * ,[  ******USE TO PROCESS DATA ON UNIT Ó  ******             ]
   * ,[  >EVALOQ FILENAME,LIBRARYLIST                             ]
   * ;[       EVALØQ QUICKLY EVALUATES THE DATA FILE FOR         ]
   * ,[       THE COMPOUNDS IN THE LIBRARY LIST  USED            ]
   * ,[       MAINLY FOR SETTING LIBRARY PARAMETERS BEFORE       ]
   * ,[       BATCH PROCESSING                                   ]
   * ,SETS NO,EDSL (-,W,E)
   * ,FILE (K PRIN 99/N,E)
   * ,SETQ TEMP,EDQL $1 (-,W,E),SETL $2
   * ;EVALÓC
   * ,EVALOD
   * ,QUAN $1 (I,F2,H,E)
   * ,EVALMO
   * ,FEED,BEEP,BEEP,BEEP
   * ,[ PROCEDURE EVALOQ IS COMPLETE ]
   *
   ERASE
   SETS NO
   EDSL  (-,W,E)
   FILE  (K PRIN 99/N,E)
   SETQ TEMP
   EDQL $1 (-,W,E)
   SETL $2
   EVALÓC
      * ,[ PART OF EVALÓ \LOCATE INTERNAL STD\ ]
      * ;SET14 #Ø
      * ,GETL
      * ,SEAR/V(I;.$,&;V4ØØØØØ;N2,1Ø,5ØØ,D-25,25,E)
      * ,EVALOF
      * ,SET1Ó !14,SETL #Ó
      *
      SET14
      GETL
      SEAR  (I,$,&;V4ØØØØØ,N2,1Ó,5ØØ,D-25,25,E)/V
      EVALOF
         * ,[ PART OF EVALO \ ?? INT  STD FOUND ?? \ ]
         * ,IF EVALOF #1,'14
         * ;PRIN(@P2),BEEP,BEEP,BEEP,BEEP
         * ,RETU EVALØB
         *
         IF EVALOF#1,'14
         PRIN  (@P2)
         BEEP
         BEEP
         BEEP
         BEEP
         RETU EVALOB
      SET1Ó !14
      SETL
   EVALOD
      * ,[ PART OF EVALÓ \DETECT SELECTED COMPOUNDS \ ]
      * ,SET1 !1Ó,SET14 #Ó
      * ,GETL
      * ;SEAR/V(I,$,%,V4ØØØØØ,N1,1Ø,1Ó,D-1Ø,1Ó,E)
      * ,PRIN/KX('4,2,'14,6,'15,6,'16,6,C,E)
      * ,EVALOG
```

```
    * ,LOOP
    *
    SET1 '1Ó
    SET14
    GETL
    SEAR  (I,$,%,V4ØÓÓØØ,N1,10,10,D-10,1Ó,E)/V
    PRIN  ('4,2,'14,6,'15,6,'16,6,C,E)/KX
    EVALÓG
       * ,[ PART OF EVALO \QUANT LOOP ENTRY\ ]
       * ,EVALOH,EDGL $1(-,N,#,A,E)
       *
       EVALÓH
          * ,[ PART OF EVALÓ \MATCH CHECK AND QUANT\ ]
          * ,[CHANGE THE NUMBER '#800' TO DESIRED LEVEL OF COMPUTER-MATCH]
          * ,IF EVALOH '16,EVALOH #600
          * ,SET1 '14
          * ,EDSL TEMP(-,'14,A,E)
          * ,EDLL $1(-,$,A,E)
          * ,EDGL(-,W,E)
          * ,CHRO(I,R,$,#,N1,2,A>5,3,G-4,4,D-10,1Ó,E)
          * ,EVALOI,RETU EVALOG
          *
          IF EVALOH'16,EVALÓH#6ÓÓ
          SET1 '14
          EDSL TEMP (-,'14,A,E)
          EDLL $1 (-,$,A,E)
          EDGL  (-,W,E)
          CHRO  (I,R,$,#,N1,2,A>5,3,G-4,4,D-1Ó,1Ó,E)
          EVALÓI
             * ;[ PART OF EVALÓ \SPECTRUM PRINTOUT\ ]
             * ,IF EVALOH '28,EVALÓH
             * ,EDGL TEMP,$1(U*20,1ÓÓ,A,E)
             * ,EDSL $1(I,-'1,4,W,E)
             * ,IF EVALÓI '27,EVALOI
             * ,LIBR(',I,N-,C,DS,HS,E)
             *
             IF EVALÓH'28,EVALÓH
             EDGL TEMP,$1 (U*2Ó,1ÓÓ,A,E)
             EDSL $1 (I,-'1,4,W,E)
             IF EVALÓI'27,EVALOI
             LIBR  (',I,N-,C,DS,HS,E)
          RETU EVALÓG
       EDGL $1 (-,N,#,A,E)
    LOOP
QUAN $1 (I,F2,H,E)
EVALMO
    * SETL #0,SET1Ó #Ó
    * ,EVALM1
    * ,CHRO(H,I,E)
    *
    SETL
    SET10
    EVALM1
       * GETL
       * ,CHRO($,K,E)
       * ,EVALM2
       * ,LOOP
       *
       GETL
       CHRO  ($,K,E)
       EVALM2
          * SET1Ó '10#1
          * ,IF '10 EVALM2,#10
          * ,CHRO(H,I,E)
          * ,SET10 #Ø
          *
```

```
            SET10 #1'10
            IF EVALM2'10,#10
            CHRO  (H,I,E)
            SET10
         LOOP
      CHRO  (H,I,E)
FEED
BEEP
BEEP
BEEP
```

```
PRINP2.ME = C20;T;                                    PRIORITY POLLUTANT EVALUATI
C;T;                        NO INTERNAL STANDARD WAS FOUND IN SAMPLE ;$1;
C;T;                                    ;D
;F;E
```

APPENDIX J

Operation of EVAL2Q

Procedure EVAL2Q

>EVAL2Q FILENAME, LIBRARY LIST is the command needed to execute the procedure.

This procedure is similar in operation to EVALØQ. The procedure is used to process data files stored on UNIT #2 of a Two-Disk-Drive System. The library list must be stored on Unit #3. Copy the library list needed from Unit #1 to Unit #3. The quantitation results generated by procedure EVAL2Q are appended to a quantitation list stored on Unit #2.

```
TRACE OF PROCEDURE EVAL2Q
   * ERASE
   * ,[ PROCEDURE EVAL2Q                                          ]
   * ,[ WRITTEN BY OJLOGSDON 1/8/80                               ]
   * ,[ BASED ON THE ORIGINAL EVALQ BY BHUGHES                     ]
   * ,[                                                           ]
   * ,[  ******USE TO PROCESS DATA ON UNIT 2  ******             ]
   * ,[  ****** LIBRARY LIST MUST BE ON 3   ********             ]
   * ,[  >EVAL2Q FILENAME,LIBRARYLIST                             ]
   * ,[       EVAL2Q QUICKLY EVALUATES THE DATA FILE FOR          ]
   * ,[       THE COMPOUNDS IN THE LIBRARY LIST  USED             ]
   * ,[       MAINLY FOR SETTING LIBRARY PARAMETERS BEFORE        ]
   * ,[       BATCH PROCESSING                                    ]
   * ,SETS 2 NO,EDSL (-,W,E)
   * ,FILE (K PRIN 99/N,E)
   * ,SETQ 2 TEMP,EDQL 2 $1 (-,W,E),SETL 3 $2
   * ,EVAL2C
   * ,EVAL2D
   * ,QUAN 2.$1 (I,F2,H,E)
   * ,EVALMØ
   * ,FEED,BEEP,BEEP,BEEP
   * ,[ PROCEDURE EVAL2Q IS COMPLETE ]
   *
   ERASE
   SETS 2 NO
   EDSL  (-,W,E)
   FILE  (K PRIN 99/N,E)
   SETQ 2 TEMP
   EDQL 2 $1 (-,W,E)
   SETL 3 $2
   EVAL2C
      * ,[ PART OF EVAL2 \LOCATE INTERNAL STD\ ]
      * ,SET14 #0
      * ,GETL
      * ,SEAR/V(I,$,&,V400000,N2,10,500,D-25,25,E)
      * ,EVAL2F
      * ,SET10 '14,SETL #0
      *
      SET14
      GETL
      SEAR  (I,$,&,V400000,N2,10,500;D-25,25,E)/V
      EVAL2F
         * ;[ PART OF EVAL2 \ ?? INT  STD FOUND ?? \ ]
         * ,IF EVAL2F #1,'14
         * ,PRIN(@P2),BEEP,BEEP,BEEP,BEEP
         * ;RETU EVAL2B
         *
         IF EVAL2F#1,!14
         PRIN  (@P2)
         BEEP
         BEEP
         BEEP
         BEEP
         RETU EVAL2B
      SET10 '14
      SETL
   EVAL2D
      * ,[ PART OF EVAL2 \DETECT SELECTED COMPOUNDS \ ]
      * ,SET1 '10,SET14 #0
      * ,GETL
      * ,SEAR/V(I,$,%,V400000,N1,10,10,D-10,10,E)
      * ,PRIN/RX('4,2,'14,6,'15,6,'16,6,C,E)
```

```
   * ,EVAL2G
   * ,LOOP
   *
   SET1 '10
   SET14
   GETL
   SEAR  (I,$,%,V400000,N1,10,10,D-10,10,E)/V
   PRIN  ('4,2,'14,6,'15,6,'16,6,C,E)/HX
   EVAL2G
      * ,[ PART OF EVAL2 \QUANT LOOP ENTRY\ ]
      * ,EVAL2H;EDGL 2,$1(-,N,#,A,E)
      *
      EVAL2H
         * ,[ PART OF EVAL2 \MATCH CHECK AND QUANT\ ]
         * ,[CHANGE THE NUMBER '#800' TO DESIRED LEVEL OF COMPUTER MATCH]
         * ,IF EVAL2H '16,EVAL2H #600
         * ,SET1 '14
         * ,EDSL 2 TEMP(-,'14,A,E)
         * ,EDLL 2 $1(-,$,A,E)
         * ,EDGL(-,W,E)
         * ,CHRO(I,R,$,#,N1,2,A>5,3,G-4,4,D-10,10,E)
         * ,EVAL2I,RETU EVAL2G
         *
         IF EVAL2H'16,EVAL2H#600
         SET1 '14
         EDSL 2 TEMP (-,'14,A,E)
         EDLL 2 $1 (-,$,A,E)
         EDGL  (-,W,E)
         CHRO  (I,R,$,#,N1,2,A>5,3,G-4,4,D-10,10,E)
         EVAL2I
            * ,[ PART OF EVAL2 \SPECTRUM PRINTOUT\ ]
            * ,IF EVAL2H '28,EVAL2H
            * ,EDGL 2 TEMP,2 $1(U*20,100,A,E)
            * ,EDSL 2 $1(I,-'1,4,W,E)
            * ,IF EVAL2I '27,EVAL2I
            * ,LIBR(',I,N-,C,DS,HS,E)
            *
            IF EVAL2H'28,EVAL2H
            EDGL 2 TEMP,2 $1 (U*20,100,A,E)
            EDSL 2 $1 (I,-'1,4,W,E)
            IF EVAL2I'27,EVAL2I
            LIBR  (',I,N-,C,DS,HS,E)
         RETU EVAL2G
      EDGL 2 $1 (-,N,#,A,E)
   LOOP
QUAN 2 $1 (I,F2,H,E)
EVALM0
   * SETL #0,SET10 #0
   * ,EVALM1
   * ,CHRO(H,I,E)
   *
   SETL
   SET10
   EVALM1
      * GETL
      * ,CHRO($,K,E)
      * ,EVALM2
      * ,LOOP
      *
      GETL
      CHRO  ($,K,E)
      EVALM2
         * SET10 '10#1
         * ,IF '10 EVALM2,#10
         * ,CHRO(H,I,E)
         * ,SET10 #0
```

```
            *
            SET10 #1'10
            IF EVALM2'10,#10
            CHR0  (H,I,E)
            SET10
         LOOP
      CHR0  (H,I,E)
FEED
BEEP
BEEP.
BEEP
```

```
PRINP2.ME = C20;T;                                    PRIORITY POLLUTANT EVALUATIC
C;T;                        NO INTERNAL STANDARD WAS FOUND IN SAMPLE ;$1;
C;T;                                    ;D
;F;E
```

APPENDIX K
Operation of MQSA
Procedure MQSA

Operation of MQSA

>MQSA FILENAME #SCAN, LIBRARY NAME, #LIBRARY ENTRY is the command needed to execute the procedure.

This procedure locates and quantitates a compound peak in a chromatographic run using the scan number and priority pollutant number read in the execution statement. The quantitation results are appended to a quantitation list with the same name as the filename. MQSA is used when EVALØQ (EVAL2Q) or EVALØ (EVAL2) fails to locate the peak of a compound that has been shown to be present after manual examination of the chromatogram.

```
TRACE OF PROCEDURE MQSA
   * ERASE
   * ;[ PROCEDURE MQSA                                                    ]
   * ;[ >MQSA FILENAME#SCAN,LIBRARY NAME,#LIBRARY ENTRY  EXECUTES         ]
   * ;[ THE PROCEDURE.                                                    ]
   * ;[                                                                   ]
   * ;[ WRITTEN BY BA HUGHES  MARCH,1980  LAST REVISION 03/21/80 BAH      ]
   * ;[                                                                   ]
   * ;[ MQSA IS A PRODEDURE THAT LOCATES AND QUANTITATES A SAMPLE         ]
   * ;[ OR STANDARD PEAK USING THE SCAN# AND PP# READ IN THE EXECUTION    ]
   * ;[ STATEMENT.  THE QUANTITATION RESULTS ARE APPENDED TO QUAN FILE    ]
   * ;[ $1.  MQSA IS USED WHEN EVALOQ (EVAL2Q) OR EVALO (EVAL2) FAILS     ]
   * ;[ TO LOCATE THE PEAK OF A COMPOUND THAT IS PRESENT.                 ]
   * ;SET4 $2
   * ;SET4 #!3
   * ;SETQ %1
   * ;CHRO(I;R;$;#;N1,2;A>5,3;G-4,4;D-10,10;H-10,10,E)
   * ;FEED;BEEP
   *
   ERASE
   SET4 $2
   SET4 !3
   SETQ $1
   CHRO  (I;R;$;#;N1,2;A>5,3;G-4,4;D-10,10;H-10,10;E)
   FEED
   BEEP
```

APPENDIX L

Operation of RFQUAL
Procedure RFQUAL
Source File for RFQUAL
Input File for RFQUAL
Typical Output of RFQUAL

>RFQUAL LIBRARY LIST is the command that executes the procedure.

This procedure initiates a FORTRAN program called RFQC, "Response Factor Quality Control". RFQC audits reference standard response factor values stored in response lists. RFQUAL is driven by a library list.

A response list for each standard compound can be created after a daily standard mixture has been quantitated and the quantitation parameters have been updated.

```
>QUAN PP1A1AJ239
QUAN: R(1,12)      Update response factors.
QUAN: S(1,12)      Update relative retention times.
QUAN: T(1,12)      Update retention times.

QUAN : <
(Write new response for each compound.)

                   or

QUAN: >
(Append each response factor to each existing response list.)
```

The procedure outputs a response list summary for each standard compound in the library list. The response list summary indicates the last response factor entered in the response list for each compound and the average and standard deviation of up to fifty response factor values in the response list. The program calculates a coefficient of variation for each compound response factor calculated. If the coefficient of variation of the response factor is greater than or equal to 30%, the response factor value is flagged and thereby brought to the attention of the analyst.

```
TRACE OF PROCEDURE RFQUAL
  * ;ERASE
  * ;[ PROCEDURE RFQUAL                                                ]
  * ;[ >RFQUAL LIBRARY LIST  IS THE COMMAND THAT INITIATES             ]
  * ;[ THE PROGRAM.                                                    ]
  *
  * ;[ OJLOGSDON AND BAHUGHES  APRIL, 1980                            ]
  * ;[ US EPA-NEIC BOX 25227 DENVER, CO 80225 303-234-4661            ]
  *
  * ;[ THIS PROCEDURE INITIATES A FORTRAN PROGRAM CALLED              ]
  * ;[ RFQC, "RESPONSE FACTOR QUALITY CONTROL". RFQC                  ]
  * ;[ EVALUATES STANDARD RESPONSE FACTOR VALUES "STORED" IN          ]
  * ;[ RESPONSE LISTS.                                                ]
  *
  * ;[ A RESPONSE LIST FOR EACH STANDARD CAN BE CREATED               ]
  * ;[ AUTOMATICALLY AFTER THE STANDARD PARAMETERS HAVE BEEN          ]
  * ;[ UPDATED.  UPDATE PARAMETERS IN QUAN.  QUAN:<  (WRITE           ]
  * ;[ NEW RESPONSE LIST.) OR  QUAN:>  (APPEND RESPONSE               ]
  * ;[ FACTORS TO EXISTING LIST.)                                     ]
  * ;ERASE
  * ;SETL $1#0
  * ;RUN RFQC
  * ;FEED
  * ;BEEP
  * ;[ PROCEDURE RFQUAL IS DONE.    ]
  *
  ERASE
  ERASE
  SETL $1
  RUN RFQC
  FEED
  BEEP
```

```
C       RFQC.FR
C       "RESPONSE FACTOR QUALITY CONTROL" FOR EVALUATION OF MULTIPLE
C       RESPONSE FACTOR VALUES CONTAINED IN RESPONSE LISTS.
C       WRITTEN BY OJLOGSON AND BAHUGHES, MARCH 1980
C       LAST REVISION  NOV 1980  BAH
C       USEPA NEIC BOX 25227 DENVER, CO. 80225  303-234-4661

        PARAMETER TTO=10, TTI=10, LPT=2, DSK=1
        PARAMETER LEN1=22, MAXQ1=50
        PARAMETER LENH=84, MAXQ2=150


        INTEGER
     1  IS(2,MAXQ2),
     1  JQ(LEN1),JFILE(11),
     1  IREPO(18,MAXQ2),
     1  DFSW,DFSW1,DFILE,SFILE

        REAL
     1  REPO(3,MAXQ2)


        COMMON /CDESC/ LDESC(11),LDESC1(11)

        COMMON /CHEAD/ NAME(35),FMASS,SMASS,IU1,IU2,
     1  LNAMER,LNUMR,NAMER(35),FMASSR,SMASSR,IU3,IU4

        COMMON /CQUAN/IDAY,IRUN,RET,METH(2),AREA,HIT,
     1  AMNT,RETR,METHR(2),AREAR,HITR,AMNTR

        EQUIVALENCE (JQ,IDAY)

        COMMON /CAREA/ IAREA(44)

        COMMON /CMAIN/
     1  NPROG,DFSW,DFSW1,ITEMP(15),
     1  DFILE(12,6),SFILE(11,4),
     1  INSTD(3),IREFTABLE(11),
     1  IADD1,IADD2,ISUB1,ISUB2,ISUB3,ISUB4,
     1  JADD1,LIBRNAME,LIBRNUMB,IBUF,
     1  ISCN(45),IACQ(100),IDAT(45)
```

```
      DATA LDESC/"D<0>",0,1,6*0,"RL",0/

      IBUF=0

C     ACCESS *.LL FILE IN CURRENT MSDS VARIABLES AND READ ENTRIES.
      DO 10 I=1,11
10    JFILE(I)=DFILE(I,2)

      N=0
      IC=0
      ICL=1
      IE=26K
      CALL FMOPS(JFILE,ICH,$8800,IEE)
      ILP=ISHFT(N,2)
      IHP=ISHFT(N,-14)
      CALL FMPOS(IHP,ILP,ICH,$8800,IEE)
      CALL FMRD(IS,ICH,MAXQ2+MAXQ2,$20,IEE)
      IEE=0

20    CALL FMCLS(ICH,$21)
21    IF (IEE.GT.0) GOTO 8800
      IC=(MAXQ2*2+IEE)/2                ,MAX # OF .RL'S.
                                        ;EQUAL TO # OF ENTRIES IN .LL .

      DO 1000 I=1,IC


      CALL CCDCZ(IFL)                   ;CHECK AND ENABLE INTERRUPT.
      IF(IFL) GOTO 5000

      DO 50 J=1,11
50    LDESC1(J)=LDESC(J)

C     CONVERT .LL ENTRY TO .RL FILENAME
      LDESC1(4)=IS(1,I)                 ;LIBRARY NAME FROM .LL ENTRY.
      N2=IS(2,I)                        ;LIBRARY ENTRY# FROM .LL ENTRY
      LDESC1(7)=0
      IBYTE=(LDESC1(4).AND.377K).EQ.0   ,ONE LETTER OR TWO?
      DO 602 J=1,5                      ;CREATE EACH DIGIT IN TURN.
      ID="<0>0"+MOD(N2,10)              ;THE APPROPRIATE DIGIT.
      IB=14+IBYTE-J                     ;BYTE POSITION IN LDESC1.
      IB1=IB.AND.1                      ;TOP OR BOTTOM OF WORD.
      IW=(IB+1)/2                       ;WORD POSITION IN LDESC1.
      LWD=LDESC1(IW)
      IF (IB1) LDESC1(IW)=(LWD.AND.377K)+ISHFT(ID,8)
      IF (IB1.EQ.0) LDESC1(IW)=(LWD.AND.177400K)+ID
602   N2=N2/10
```

```
C       ACCESS .RL DATA FILES
        JC=0
        SUM=0.0
        SUMSQ=0.0
        IE=34K

        WRITE(TTO,2) (LDESC1(J),J=4,9)
 2      FORMAT(1X,"PROCESSING LIST:  ",A2,",",6A2)

        DO 30 J=1,15
 30     IREPO(J,I)="   "

        CALL FMOPS(LDESC1,ICH,$500,IEE)
        IE=40K
        CALL FMRD(NAME,ICH,LENH,$100,IEE)
 55     CALL FMRD(JQ,ICH,LEN1,$100,IEE)

C       JC=N                        ;NUMBER OF RESPONSE FACTORS ACCESSED.
        JC=JC+1

        REF=(AREA/AREAR)*(AMNTR/AMNT)+.0005    ;CALCULATE RESPONSE FACTOR.
        SUM=SUM+REF
        SUMSQ=SUMSQ+REF*REF

        IF (JC.LE.MAXQ1) GOTO 55
        WRITE (TTO,65) JC
 65     FORMAT(" MORE THAN "I4" ENTRIES IN RESPONSE LIST")
        GOTO 550
 100    IF (IEE.NE.-LEN1) GOTO 8800
        CALL FMCLS(ICH,$8800)

C       CALCULATE AVERAGE,STANDARD DEVIATION.
C       I=INDEX NUMBER OF .RL ENTRY.

        DO 200 J=1,15
 200    IREPO(J,I)=NAME(J)          ;30 CHARACTERS OF NAME.

        IF (JC.GT.1) GOTO 300
 250    IREPO(16,I)=-1
        IREPO(17,I)=IS(1,I)
        IREPO(18,I)=IS(2,I)
        GOTO 400

 300    MASS=FMASS+SMASS
        MASS=(MASS+1)/2
        IREPO(16,I)=MASS            ;QUANTITATION MASS
        IREPO(17,I)=IS(1,I)         ;LIBRARY NAME.
        IREPO(18,I)=IS(2,I)         ;LIBRARY ENTRY NUMBER
        REPO(1,I)=SUM/JC            ;AVERAGE RESPONSE FACTOR.
        REPO(2,I)=SQRT(ABS(SUMSQ-SUM**2.0/JC)/(JC-1))
                                    ;STD DEVIATION.
        REPO(3,I)=REF               ,LAST ENTRY TO RESPONSE LIST(CURRENT RESP)
 400    GOTO 1000
 500    IF(IEE.NE.22K) GOTO 8800
        GOTO 250

 550    IREPO(16,I)=-2
        IREPO(17,I)=IS(1,I)
        IREPO(18,I)=IS(2,I)


1000    CONTINUE
```

```
        CALL OPLPT(ICH,$8800)

C       WRITE REPORT HEADER.

        CALL GETTI(IYR,IMO,IDAY,IHR,IMIN,ISEC,$1170,IX,IX,IX,IX,IX,IX)
1170    IYR=IYR-IYR/100*100
        WRITE(ICH,1180)(JFILE(J),J=4,9),IMO,IDAY,IYR
1180    FORMAT(1X,8X,"RESPONSE LIST SUMMARY FOR ENTRIES IN LIBRARYLIST: ",
     1  6A2,4X,I2,"/",I2,"/",I2,/)
        WRITE(ICH,1190)
1190    FORMAT(1X,50X,"RESPONSE FACTORS")
        WRITE(ICH,1200)
1200    FORMAT(1X,15X,"NAME",15X,"LIB#",3X,"M/E",3X,"AVG",3X,"STDDEV",
     1  2X,"CV%",2X,"RESP")

C       WRITE REPORT.

        DO 2000 I=1,IC
        CALL CCDCZ(IFL)
        IF (IFL) GOTO 4000
        IFLAG="  "
        IF (IREPO(16,I).GT.0) GOTO 1300
        IFLAG="NA"
        IF(IREPO(16,I).EQ.-2) IFLAG="XS"
        WRITE(ICH,1310) (IREPO(J,I),J=1,15),IREPO(17,I),IREPO(18,I),IFLAG
1310    FORMAT(1X,15A2,T35,A2,",",I3,T81,A2)
        GOTO 2000

1300    CV=REPO(2,I)*100.0/REPO(1,I)
        IF (CV.GE.30.0) IFLAG="**"

        WRITE(ICH,1500) (IREPO(J,I),J=1,15),IREPO(17,I),IREPO(18,I),
     1  IREPO(16,I),REPO(1,I),REPO(2,I),CV,REPO(3,I),IFLAG
1500    FORMAT (1X,15A2,T35,A2,",",I3,2X,I3,2(2X,F5.3),
     1  2X,F4.1,2X,F5.3,1X,A2)

2000    CONTINUE

        WRITE(ICH,2500)
2500    FORMAT(1X,"_____",///,1X,
     1  "CV%=COEFFICIENT OF VARIATION (STDDEV*100/AVG).",/,1X,
     1  "NA=NOT ENOUGH DATA.",/,1X,
     1  "XS=MORE THAN 50 DATA POINTS.",/,1X,
     1  "RESP=CURRENT RESPONSE FACTOR.",/,1X,
     1  "**=OUTSIDE OF CONTROL LIMITS.")


4000    WRITE(ICH,4100)
4100    FORMAT (" <14>")
5000    CALL FMCLS(ICH,$8800)

6000    CALL LOADIT("EXEC")

8800    WRITE (TTO,8810) IE,IEE
8810    FORMAT(" IDOS ERROR"/
     1  " OPERATION "OI3" CODE "OI6)
        GOTO 6000
        END
```

```
[ INPUT FILE  RFQC.IN, USE TO LOAD  RFQC.RB .]
[ +IN RFQC.IN  EXECUTES THE FILE.            ]
GL
L/F CMAIN+MFLIB+RFQC+MEMLM+FMRD+FMCLS+OPLPT+FMOPN+FMPOS+ISHFT+TIMER
M/TU
S/F 1:RFQC.MS,CAREA:.END
E
```

Typical output for RFQUAL

RESPONSE LIST SUMMARY FOR ENTRIES IN LIBRARYLIST: PPPH 11/ 6/80

	NAME	LIB#	M/E	RESPONSE FACTORS AVG	STDDEV	CV%	RESP
ISA	D10-PHENANTHRENE	PP, 133	188	1.000	0.002	0.2	1.000
21	2,4,6-TRICHLOROPHENOL	PP, 21	196	0.201	0.057	28.4	0.213
22	4-CHLORO-3-METHYLPHENOL	PP, 22	142	0.343	0.046	13.6	0.324
24	2-CHLOROPHENOL	PP, 24	128	0.511	0.076	14.8	0.442
31	2,4-DICHLOROPHENOL	PP, 31	162	0.416	0.070	16.9	0.473
34	2,4-DIMETHYLPHENOL	PP, 34	122	0.334	0.054	16.2	0.253
57	2-NITROPHENOL	PP, 57	139	0.267	0.054	20.5	0.267
58	4-NITROPHENOL	PP, 58	139	0.056	0.017	30.6	0.050
59	2,4-DINITROPHENOL	PP, 59	154	0.022	0.004	19.0	0.017
60	4,6-DINITRO-O-CRESOL	PP, 60	198	0.056	0.004	8.2	0.061
64	PENTACHLOROPHENOL	PP, 64	266	0.062	0.002	4.8	0.058
65A	PHENOL	PP, 65	94	0.594	0.138	23.3	0.435
ISA	D8-NAPHTHALENE (135)	PP, 135	136	1.279	0.167	13.1	1.128

CV%=COEFFICIENT OF VARIATION (STDDEV*100/AVG).
NA=NOT ENOUGH DATA.
XS=MORE THAN 50 DATA POINTS.
RESP=CURRENT RESPONSE FACTOR.
**=OUTSIDE OF CONTROL LIMITS.

APPENDIX M

Operation of Procedure EVALSP

Procedure EVALSP

>EVALSP,, LIBRARYLIST is the command that activates the procedure.

This procedure prints a copy of the mass spectrum of each library entry listed in the library list. The procedure facilitates the compilation of standard compound reference spectras.

```
TRACE OF PROCEDURE EVALSP
   * ERASE
   * ;[ PROCEDURE EVALSP                                              ]
   * ,[ WRITTEN 10/22/79 BY D A  HUGHES,                              ]
   * ;[ US EPA - NEIC   303-234-4661                                   ]
   * ,[ MODIFIED - DAH 01/10/80                                       ]
   * ;[                                                               ]
   * ,[ THIS PROCEDURE COPIES THE SPECTRUM OF EACH                     ]
   * ,[ LIBRARY ENTRY LISTED IN THE LIBRARY LIST.                      ]
   * ;[                                                               ]
   * ;[ SET ANY OPERATING DATAFILE IN $1,CALFILE IN $2                 ]
   * ;[                                                               ]
   * ;[ :EVALSP,,LIBRARYLIST  IS THE COMMAND NEEDED TO                 ]
   * ,[ ACTIVATE THE PROCEDURE                                         ]
   * ;[ THE LIBRARYLIST IS STORED IN $3                               ]
   * ;[                                                               ]
   * ;[                                                               ]
   * ;SETL $3
   * ;EDLL(D,E)
   * ;EVALS1
   * ;BEEP,BEEP:BEEP
   * ,ERASE
   * ;[ PROCEDURE EVALSP IS DONE ]
   *
   ERASE
   SETL $3
   EDLL  (D,E)
   EVALS1
      *
      * ,[ PART OF EVALSP \GET LIBRARY ENTRY, COPY\ ]
      * ;GETL
      * ;LIBR$1#100(I,G;F,HS,E)
      * ;LOOP
      *
      GETL
      LIBR$1 #100 (I,G,F,HS,E)
      LOOP
   BEEP
   BEEP
   BEEP
   ERASE
```

APPENDIX N

Operation of Procedure EVALLB

Procedure EVALLB

>EVALLB,,LIBRARYLIST is the command that initiates the procedure.

This procedure prints a copy of the library parameters and the mass/intensity data of each compound referenced in the library list. The procedure facilitates the compilation of standard compound reference mass/intensity data in tabular form.

```
TRACE OF PROCEDURE EVALLB
   * ERASE
   * ;[ PROCEDURE EVALLB                                                ]
   * ;[ WRITTEN 01/11/80 BAH                                           ]
   * ,[ US EPA - NEIC  303-234-4661                                     ]
   * ;[                                                                 ]
   * ;[ THIS PROCEDURE COPIES THE LIBRARY PARAMETERS OF EACH           ]
   * ,[ COMPOUND REFERENCED IN THE LIBRARY LIST                         ]
   * :[                                                                 ]
   * ,[ SET ANY OPERATING DATAFILE IN $1, CALFILE IN $2                 ]
   * ,[                                                                 ]
   * ;[ EVALLB.,LIBRARYLIST  IS THE COMMAND NEEDED TO                   ]
   * ,[ ACTIVATE THE PROCEDURE.                                         ]
   * :[ THE LIBRARY LIST IS STORED IN $3                                ]
   * ;[                                                                 ]
   * ;[                                                                 ]
   * ;SETL $3
   * ,EDLL (B,E)
   * ,EVALL1
   * ;BEEP,BEEP,BEEP
   * ;ERASE
   * ;[ PROCEDURE EVALLB IS DONE ]
   *
   ERASE
   SETL $3
   EDLL  (B,E)
   EVALL1
      * ;[ PART OF EVALLB \GET LIBRARY ENTRY, COPY PARAM\  ]
      * ;GETL
      * ;EDLB (H,E)
      * ,LOOP
      *
      GETL
      EDLB  (H,E)
      LOOP
   BEEP
   BEEP
   BEEP
   ERASE
```

APPENDIX O

Operation of Procedure Disk

Procedure Disk

Source File for Disk

Input File for Disk

Typical Output from Disk

>DISK# (i.e., DISK #5 where 5 is the number assigned to the disk pack) executes this procedure. One must also input the unit number of the disk drive where the disk pack is loaded.

This procedure prints a report of the filename type stored on the disk pack and disk drive unit referenced in the execution statements. The report indicates the date and time the procedure DISK was executed and the space available on the disk pack at that time. The information written under the headings, "Filename", "Date", "Length" is the information stored in MSDS procedure FILE. The information written for each filename under the heading "Sample Description" is the information entered in ACQUIRE/accounting mode in the slot SAMPLE.

```
TRACE OF PROCEDURE DISK
   * SET3 #99,ERASE,
   * ;[ PROCEDURE DISK                                                    ]
   * ;[ WRITTEN BY OJ LOGSDON  FEB,1980                                   ]
   * ;[ US EPA-NEIC  303-234-4661                                         ]
   * ;[                                                                   ]
   * ;[ >DISK#   EXECUTES THIS PROCEDURE.  (IE,>DISK#5)                   ]
   * ;[ TIME MUST BE SET.                                                 ]
   * ;[ INPUT THE UNIT NUMBER WHERE THIS DISK RESIDES                     ]
   * ,[  TYPE.  SET3 #0  OR  SET3 #2     (#0 OR #2 ONLY)                 ]
   * ;PAUSE.SETN DISKFILES;DISK1,ERASE.BEEP,BEEP;BEEP
   * ;[INVALID UNIT NUMBER, ONLY #0 OR #2 PLEASE]
   *
   SET3 #99
   ERASE
   PAUSE
   SETN DISKFILES
   DISK1
      * DISK2,FILE(D0.*;<;E);RUN LOG,FEED,BEEP;QUIT
      *
      DISK2
         * IF '3 DISK2,DISK2
         * ,IF !3 DISK1,#1! DISK1
         * ,IF #3 DISK1,!3 DISK1
         * ;FILE(D2.*,<,E),RUN LOG;FEED,BEEP,,ERASE,QUIT
         *
         IF DISK2'3,DISK2
         IF DISK1!3,DISK1#1
         IF DISK1#3,DISK1!3
         FILE  (D2:*;<,E)
         RUN LOG
         FEED
         BEEP
         ERASE
         QUIT
         TRACE OF DISK2 ABORTED.
      FILE  (D0:*;<,E)
      RUN LOG
      FEED
      BEEP
      QUIT
      TRACE OF DISK1 ABORTED.
   ERASE
   BEEP
   BEEP
   BEEP
```

```
C       DATA FILE LOG(PRINTOUT FOR INCOS SYSTEM
C       WRITTEN 2/16/80 BY OJLOGSDON  EPA/NEIC  303-234-4661
C       THIS PROGRAM RUNS IN MSDS AND OUTPUTS DATA FILE
C       INFORMATION FOR FILES IN THE CURRENT MSDS NAMELIST

        PARAMETER TTO=10
        PARAMETER MAXN=100                ;MAXN IS MAXIMUM NO. OF FILES

        INTEGER IS(11,MAXN),JFILE(11,2)

        EQUIVALENCE
     1  (IP1,ITEMP(4)),
     1  (IP2,ITEMP(5)),
     1  (JFILE,IAREA)

        COMMON /CAREA/ IAREA(2000)        ;LEAVE DATA AREA ALONE

        INTEGER
     1  INST(3),SAMPLE(32),DATE(4),RUNTIME,ANALIST(4),
     1  FORMULA(10),ICONDITIONS(32),SUBMITTED(4),ACCOUNT(4),
     1  NCALIB(11),NDATAF(11),
     1  DFSW,DFSW1,DFILE,SFILE,
     1  HIMASS,SCNFCN,THRESHOLD,
     1  SAMPINT,BASE,HIREF,UPSCAN

        COMMON /CMAIN/
     1  NPROG,DFSW,DFSW1,ITEMP(15),
     1  DFILE(12,6),SFILE(11,4),
     1  INSTD(3),IREFTABLE(11),
     1  IADD1,IADD2,ISUB1,ISUB2,ISUB3,ISUB4,
     1  JADD1,LIBRNAME,LIBRNUMB,IBUF,
     1  ISCN(45),IACQ(100),IDAT(45)

        EQUIVALENCE
     1  (ITEMP1,ITEMP),
     1  (ITEMP14,ITEMP(14)),
     1  (ITEMP15,ITEMP(15))
```

```
C       FOR SCAN PARAMETERS
        EQUIVALENCE
     1  (NDATAF, ISCN(1)),          ;ORIG DATA FILE NAME
     1  (LOWMASS, ISCN(12)),        ;LOW MASS FOR SCAN
     1  (HIMASS, ISCN(13)),         ;HI MASS FOR SCAN
     1  (UPTIME, ISCN(14)),         ;UPSCAN TIME (IN SECS)
     1  (DOWNTIME, ISCN(16)),       ;DOWNSCAN TIME (IN SECS)
     1  (TOPHOLD, ISCN(18)),        ;HOLD TIME AT TOP (SECS)
     1  (BOTTOMHOLD, ISCN(20)),     ;HOLD TIME AT BOTTOM (SECS)
     1  (SCNFCN, ISCN(22)),         ;SCAN FUNCTION FOR ACQUISITION SCAN
     1  (IACCVOL, ISCN(23)),        ;ACCELERATING VOLTAGE
     1  (ITCON, ISCN(24)),          ;ACQUISITION CONTROL WORD
     1  (JADCS, ISCN(25)),          ;ADC SAMPLING INT  (MU-SECS)
     1  (NPT, ISCN(26)),            ;HARDWARE ADD COUNT
     1  (JIOND, ISCN(27)),          ;INTENSITY/ION
     1  (NSAMP, ISCN(28)),          ;SOFTWARE ADD COUNT
     1  (UPSCAN, ISCN(29)),         ;ACQUISITION DIRECTION (-1=UP, 0=DOWN)
     1  (INST, ISCN(30)),           ;INSTRUMENT NAME (6 CHARS)
     1  (RESOLUTION, ISCN(33)),     ;RESOLUTION OR PEAK WIDTH
     1  (THRESHOLD, ISCN(35)),      ;A/D THRESHOLD
     1  (MRATE, ISCN(36)),          ;MASTER RATE
     1  (SAMPINT, ISCN(37)),        ;HARWARE SAMPLING INTERVAL (MU-SECS)
     1  (MAREA, ISCN(38)),          ;MINIMUM AREA
     1  (MINWIDTH, ISCN(39)),       ;MINIMUM PEAK WIDTH
     1  (MINFW, ISCN(40)),          ;MINIMUM FRAGMENT WIDTH AS % OF SAMP/PEAK
     1  (IBSLN, ISCN(41)),          ;BASELINE TO SUBTRACT
     1  (ISAT, ISCN(42)),           ;SATURATED VALUE
     1  (ITRLR, ISCN(43)),          ;SCAN TRAILER DESCRIPTION
     1  (MZERO, ISCN(44)),
     1  (MFULL, ISCN(45))

C       FOR ACQUISITION PARAMETERS
        EQUIVALENCE
     1  (DATE, IACQ(1)),            ;DATE OF ACQUISITION
     1  (RUNTIME, IACQ(5)),         ;TIME ACQU STARTED (AS H*100 + M)
     1  (NSCANS, IACQ(6)),          ;NUMBER OF SCANS
     1  (MSCANS, IACQ(7)),          ;NUMBER OF 1ST SCAN WITH DATA
     1  (WEIGHT, IACQ(8)),          ;ACCOUNTING QUESTIONS
     1  (SAMPLE, IACQ(10)),
     1  (ICONDITIONS, IACQ(42)),
     1  (SUBMITTED, IACQ(74)),
     1  (ANALIST, IACQ(78)),
     1  (ACCOUNT, IACQ(82)),
     1  (FORMULA, IACQ(86))
```

```
C       FOR ACCUMULTED INFO.
        EQUIVALENCE
      1 (MINAREA, IDAT(1)),       ;MINAREA AFTER READ
      1 (MERGE, IDAT(2)),         ;MERGE TO AS % OF RES
      1 (IATOL, IDAT(3)),         ;ALIGN TOL (ADD AND SUBTR)
      1 (ITOL, IDAT(4)),
      1 (LASTPEAKS, IDAT(5)),     ;MAX PEAKS TO READ IN
      1 (IDEF, IDAT(6)),          ;MASS DEF AT 100 AMU IN MMU
      1 (INOCT, IDAT(8)),         ,NOISE REJ FOR ENHA
      1 (ICUCT, IDAT(9)),         ;TAIL REJ FOR ENHA
      1 (IBKCT, IDAT(10)),        ;MAX DACKGROUND INTERVAL FOR ENHA
      1 (SCNRATIO, IDAT(11)),     ;MULT BACK BY A FACTOR OF IN ADD
      1 (JSAMPINT, IDAT(25)),     ;CALI SAMPINT
      1 (JRATE, IDAT(26)),        ;CALIBRATION RATE
      1 (JACCVOL, IDAT(27)),      ;CALI ACC VOL
      1 (LOWREF, IDAT(28)),       ;LOW REF MASS,  CALIB DATA
      1 (HIREF, IDAT(29)),        ;HIGH REF MASS
      1 (NUMREF, IDAT(30)),       ;COUNT OF REF PEAKS KNOWN
      1 (JSCAN, IDAT(31)),        ;CALI SCAN #
      1 (NCALIB, IDAT(32)),       ;CALIBRATION TALBLE NAME
      1 (BASE, IDAT(43)),         ;BASE INDEX, COMPUTED VALUES
      1 (ITOT, IDAT(44)),         ;TOT ION
      1 (LASTPEAK, IDAT(45))      ;PEAK COUNT
```

```
        WRITE(TTO) "DATA FILE LOG PRINTING"

C       OPEN AND READ THE CURRENT MSDS NAMELIST
        DO 10 I=1,11
10      JFILE(I,1)=DFILE(I,1)
        CALL FMOPN(JFILE,ICH,$8000,IEE)
        IE=40K
        CALL FMRD(IS,ICH,11*MAXN,$20,IEE)
        IEE=0
20      CALL FMCLS(ICH,$21)
21      IF (IEE.GT.0) GOTO 8000
        IC=(11*MAXN+IEE)/11
        IBUF=0

C       OPEN THE PRINTER AND OUTPUT DATE AND UNIT HEADERS
C       DISC PACK NO. IS IN !1 AND UNIT NO. IS IN !3
        CALL OPLPT(KCH,$9000)
        CALL GETTI(IYR,IMO,IDAY,IHR,IMIN,ISEC,$40,IX,IX,IX,IX,IX,IX)
40      IYR=IYR-IYR/100*100
        WRITE(KCH,50)IADD1,JADD1,IMO,IDAY,IYR,IHR,IMIN,ISEC
50      FORMAT(/"   INCOS DISC PACK NO. "I2"  CURRENTLY ON UNIT NO. "
     1  I2,T60"DATE      "I2"/"I2"/"I2"    "I2":"I2":"I2)
        ITOT=9792
        CALL ACQSPC(IFREE,JADD1,IE,IEE)
        IF (IEE.GT.0) GOTO 8000
        WRITE(KCH,65)IFREE,ITOT
65      FORMAT(1X,T20,I4" SECTORS AVAILABLE OF "I4" TOTAL"//)
        WRITE(KCH,75)
75      FORMAT(3X"FILENAME"T22"DATE"T31"LENGTH"T50"SAMPLE DESCRIPTION"/)

C       LOOP FOR LOOKING AT EACH DATA FILE HEADER FOR INFORMATION
        DO 1000 I=1,IC
        CALL CCDCZ(IFL)          ;ALLOW CRTL CHARACTERS TO INTERUPT
        IF (IFL) GOTO 1200
        DO 100 J=1,11            ;SETUP THE NEXT DATAFILE NAME
100     JFILE(J,1)=IS(J,I)
C       OPEN AND GET THE HEADER DATA FROM THE FILE
        CALL FMOPN(JFILE,ICH,$8000,IEE)
        IE=40K
        CALL FMRD(ISCN,ICH,190,$120,IEE)
        IEE=0
120     CALL FMCLS(ICH,$121)
121     IF (IEE.GT.0) GOTO 8000
        CALL GTSCN(NSCANS,JFILE,$8000,IE,IEE)
        WRITE(KCH,500) (JFILE(J,1),J=4,10),DATE,NSCANS,SAMPLE
500     FORMAT(2X,6A2",  "A2,T20,4A2,T32,I4,T40,32A2)
1000    CONTINUE
```

```
C       CLOSE THE PRINTER AND WRITE OUT FF
1200    WRITE(KCH,1500)
1500    FORMAT(" <14>")
        CALL FMCLS(KCH,$8000)

C       RETURN TO MSDS
7000    CALL LOADIT("EXEC")

C       ERROR RETURNS FOR I/O AND PRINTER
8000    WRITE(TTO,8001) IE,IEE
8001    FORMAT(" IDOS ERROR"/
     1  " OPERATION"OIJ" CODE"OI6)
        GOTO 7000
9000    WRITE(TTO,9001)
9001    FORMAT(" PRINTER BUSY OR NOT READY")
        GOTO 7000

        END
```

```
[ INPUT FILE  LOG IN ,  USE TO LOAD  LOG RB          ]
GL
L/F CMAIN+MFLIB+LOG+FMOPN+FMRD+FMCLS+OPLPT+GTSCN+TIMER+ACQSPC
M/TU
S/F 1.LOG MS.CAREA:.END
E
```

Appendix 04. Typical Output from DISK

```
INCOS DISC PACK NO   6  CURRENTLY ON UNIT NO   2        DATE      5/27/80   16 55 53
                348 SECTORS AVAILABLE OF 9792 TOTAL

 FILENAME          DATE      LENGTH            SAMPLE DESCRIPTION

624O1ACDU TI      04/29/80.    600    624-01 ACID EXT DUPLICATE 100%1ML IS3A1A 40NG/UL 2UL
624O1ACSA TI      04/29/80     600    624-01 ACID EXT ORIG WATER SAMPLE IS3A1A 40NG/UL 2UL
624O1ACSP TI      04/29/80     600    624-01 ACID SPIKE W SM101A 1ML 100%1ML IS3A1A 40NG/UL 2UL
624O2ACSA TI      04/28/80     633    624-02 ACID SAMPLE 100%1ML IS3A1A 40NG/UL 2UL
624O3ACSA TI      04/29/80     600    624-03 ACID EXT WATER SAMPLE IS3A1A 40NG/UL 100%1ML 2UL
624O4ACSA TI      04/29/80     600    624-04 ACID EXT 100%/1ML IS3A1A 40NG/UL 2UL SU201A 300NG/UL
624O5ACSA1 TI     04/30/80     600    624-05 ACID REPEAT RUN 100%1ML
624O6ACSA TI      04/30/80     610    624-06 ACID WATER SAMPLE 100%/1ML IS3A1A 40NG/UL 2UL
624XXACBL TI      04/28/80     611    624 ACID METHOD BLANK W/SU201A ADDED 100,300NG/UL IS3A1A 40NG/UL
CO428A CT         04/28/80       1    DFTPP 100NG
CO428A TI         04/28/80       3    DFTPP 100NG
CO429A CT         04/29/80       1    0
CO429A TI         04/29/80       3    0
CO430B CT         04/30/80       1    0
CO430B TI         04/30/80       3    0
DFTPP430 TI       04/30/80     156    DFTPP 50NG
DFTPPJ237 TI      04/28/80     224    DFTPP 100NG
DFTPPJ238 TI      04/28/80     173    DFTPP 100NG
DFTPPJ245 TI      04/29/80     173    0
PP1A1AJ239 TI     04/28/80     612    PP1A1A WITH IS3A1A 40NG/UL 2UL
PP1A1AJ246 TI     04/29/80     653    PP1A1A WIS3A1A 40NG/UL 2UL
PP1A2A430 TI      04/30/80     600    PP1A2A WITH IS3A1A 40NG/UL 2UL
SU201A TI         04/29/80     600    SU201A WIS3A1A 40NG/UL 300NG/UL A,A,A TRI F
SU201A430 TI      04/30/80     600    SURROGATE SPIKE 100,300 W IS3A1A 40NG/UL 2UL
```