2021 CDS GC/MS LIBRARIES

The CDS Library disk now contains several different libraries in multiple formats. These libraries are intended to be used in two different applications - Pyrogram searching by averaging all the spectra in a pyrogram and Additives to search a pyrogram for specific additives or the individual pyrolysis products of additives.

PYROGRAM SEARCHING

The PYROLYSIS LIBRARY is a collection of over 560 spectra generated by averaging all of the spectra in a pyrogram so that the standard GC/MS software can be used to identify unknowns. To use it, the spectra of the entire chromatogram is averaged. The resulting spectrum does not represent one compound, but rather contains information from all the peaks and therefore is used toidentify the polymer, not just one compound from the polymer.

ADDITIVE

ADDITIVE libraries are available in formats for AMDIS, NIST and ChemStation. The AMDIS program (available freeonline http://www.amdis.net/) is used to identify specific peaks in a complex pyrogram. The program identifies individual components in a complex chromatogram, and the spectra in each component are searched against a library of compounds (for example, plasticisers) and then peaks are indicated which may be those specific compounds. The CDS libraries, which include additives and lignocellulosic contain over 570 entries.

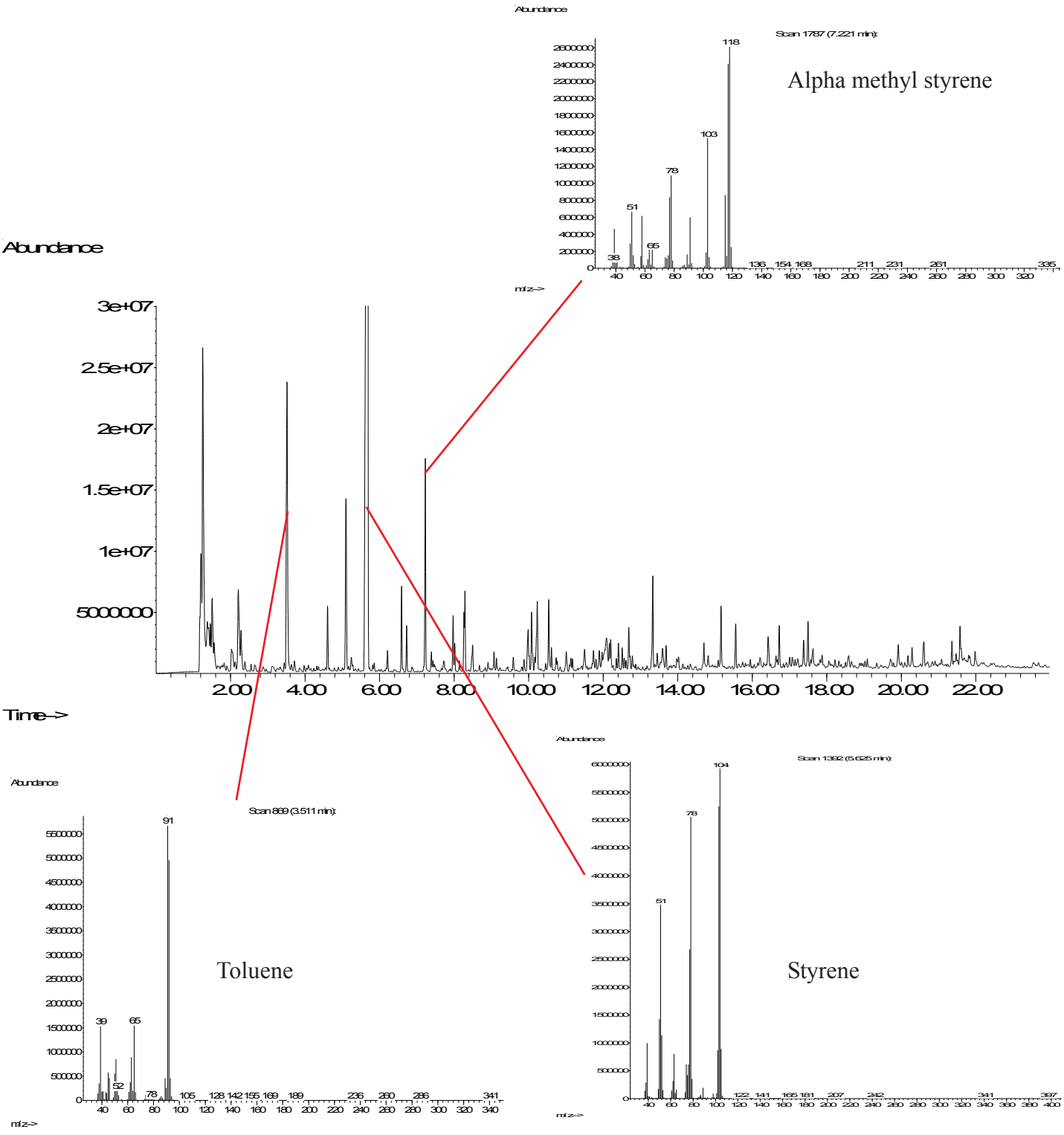
This gives the analyst three GC/MS techniques to use in studying an unknown using pyrolysis. First, the sample is pyrolyzed, and the resulting pyrogram peaks are analyzed by the GC/MS in the same way used for any other chromatogram. The individual peaks in the pyrogram may be identified using standard GC/ MS libraries.

Second, the whole pyrogram may be averaged and searched using the pyrolysis library from CDS, which has hundreds of polymers averaged to one spectrum.

Third, the pyrogram may be deconvoluted to find small amounts of specific compounds (like additives) using the additive libraries in conjuction with AMDIS.

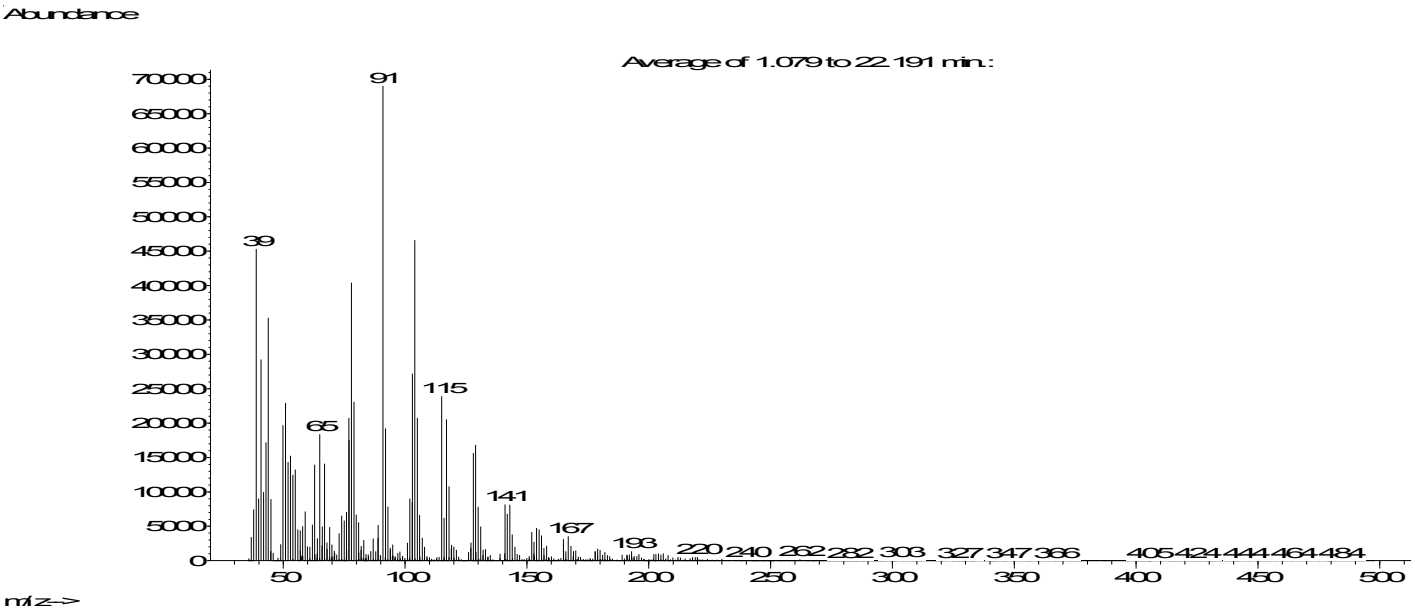
PYROGRAM SEARCHING

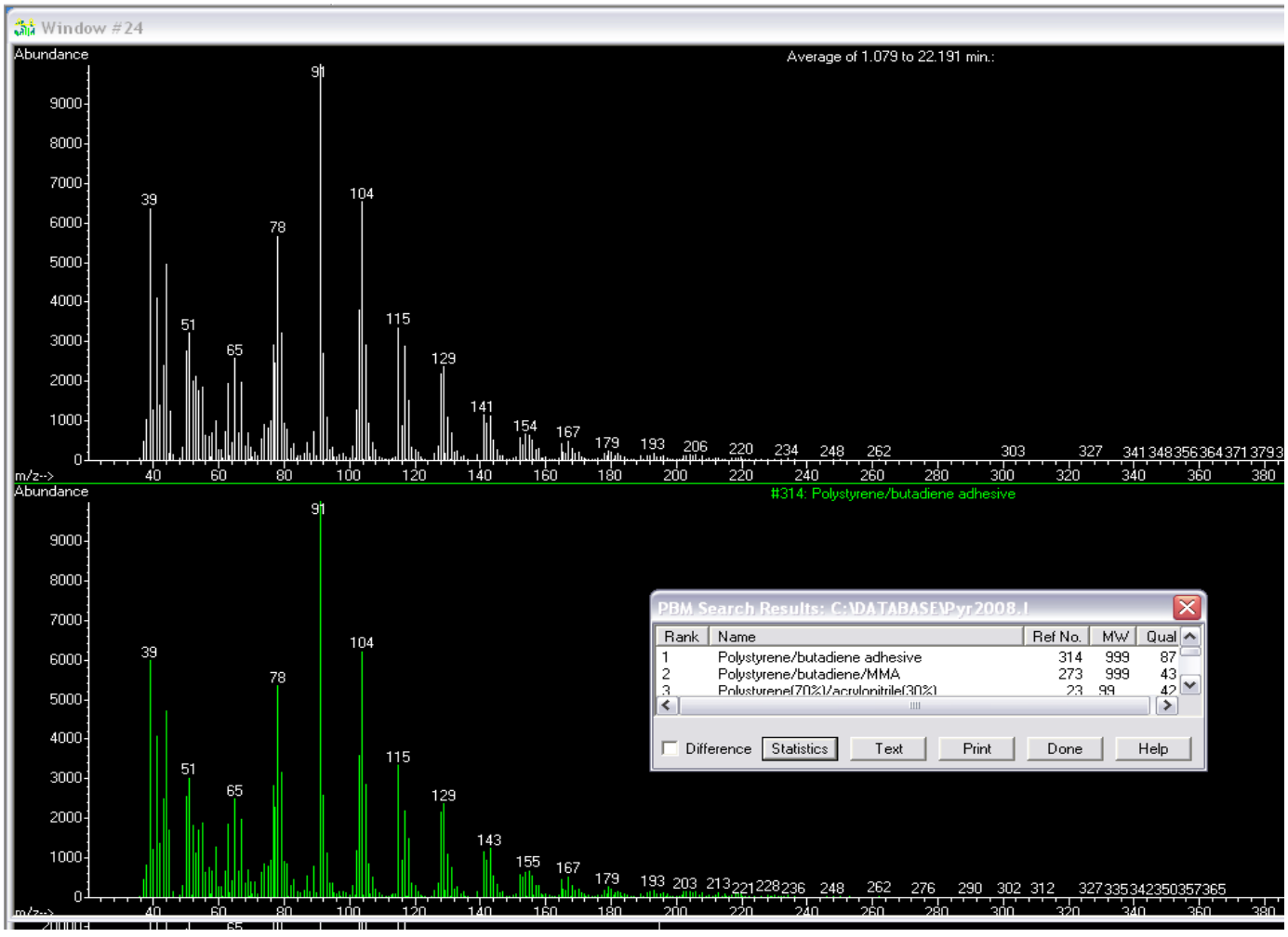
Py-GC/MS creates a chromatogram of the degradation products of the polymeric sample. Using standard searching, the individual peaks may be identified, as below.



PYROGRAM SEARCHING

If the mouse button is held down and the cursor dragged across the entire pyrogram, an average spectrum is produced for the whole run, with masses from all the peaks in the pyrogram. This spectrum is then searched against the pyrolysis library which has spectra generated the same way for known polymers.





This uses the regular GCMS software to search the unknown, in this case, a styrene/butadiene rubber.

LIST OF MATERIALS IN THE CDS PYROLYSIS LIBRARY (Some duplicate material names may exist due differing formulations of the material)

16% PE in PP
25% PE in PP
2-Ethyl hexyl acrylate
7% PE in PP
9% PE in PP
Abieta DR 835A Rosin
Acrylic (2-EHA, 2-EHMA)
Acrylic (BA,EHA)
Acrylic (EA, EMA)
Acrylic (EA,MMA, EMA)
Acrylic (MMA, BA, BMA)
Acrylic (MMA, BA, BMA, HydroxypropylMA)
Acrylic (MMA, BA, BMA, MAA)
Acrylic (MMA, BA, Hydroxy ethylMA)
Acrylic (MMA, BA, IPMA)
Acrylic (Styrene, BA, BMA)
acrylic adhesive, phthalate
Acrylic urethane epoxy polyester powdercoat
Acrylonitrile Thermoset
Acrylonitrile thermoset with plasticizer
Adhesive (Polyisobutylene, propylene, styrene) - Tape
Adhesive, from clear tape
Adhesive, hot melt
Adhesive, label
Adhesive, press sensitive
Adhesive, tacky – insert in publication
Adhesive, temporary – from "Press-Apply" label
Adhesive, temporary – Post-It flag
Adhesive, temporary, magazine insert
Alkyd paint
Alpha cellulose
Amber (Baltic)
Amber (Burma)
Amber (Jordan)
Amber (Lebanon)
Anox 20 (antioxidant)
Aramide fiber
Asphalt residue
Asphalt, modified
Asphalt, polymer modified
Asphaltene
Bamboo fiber
Beeswax 2
Beeswax EGA 100C per min 100 to 800
Beeswax Sample 1
Beeswax Sample 2
Beeswax, HMDS treated
Beeswax Sample 1
Beeswax Sample 2
Beeswax, HMDS treated
Biomass (Aspen)
Biomass (Corn stover)
Biomass (Pine Wood)
Biomass Arabidopsis
Biomass Sorgum
BisPhenol A Epoxy Uncured
Bitumen
Black Spray paint (Krylon)
Black spray paint (Rustoleum)
Blister Pack
blue foam EGA
Blue pigment (PB15)
Brake lining Phenolic
Brown Suede with phthalate
Butvar
Butyl Rubber
Calcium stearate
Candiililla Wax
Canola Oil
Carboxymethyl cellulose
Carnauba Wax
Carpet Fiber (Nylon 6)
Carpet Fiber (Nylon 6/6)
Cellulose
Cellulose acetate
Cellulose acetate (with DEP)
Cellulose propionate
Chewing gum with glycerine
Chewing gum with sugar
Chewing gum, mint
Chimassorb 119 (antioxidant)
Chimassorb 944 antioxidant
Chitin Sample 1
Chitin Sample 2
Chitosan Sample 1
Chitosan Sample 2
Circuit board plastic
Circuit board polymer
clear lens cover lid (polycarbonate) EGA
Clear tape – E-Z brand, tape only
Clear tape with adhesive and plasticizer
coal EGA
Collagen Types 1 & 3
Copal
Copal (Brazil)

Cotton, white
Crude oil Sample 1
Crude oil Sample 2
Crude oil Sample 3
Cupuacu Butter
Cupuacu Butter 2
Cutting oil
Damar (Kremmer)
Dextrose
disposable food container (PET) EGA
Dried linseed oil
Dried poppyseed oil
Dried tung oil
Eastman Poly Pale Rosin
Elastalon tubing
Elvanol 50-42 (88% hydrolyzed Polyvinyl Alcohol)
Elvanol 71-30 (fully hydrolyzed Polyvinyl Alcohol)
Enamel paint (with polyurethane)
EPDM Rubber
Epoxy adhesive (Cured)
Epoxy clear coat
Epoxy clear coating Sample 1
Epoxy clear coating Sample 2
Epoxy clear coating Sample 3
Epoxy clear coating Sample 4
Epoxy clear coating with styrene
Epoxy composite
Epoxy cured (Weldbond)
Epoxy paint
Epoxy polyester hybrid powdercoat Sample 1
Epoxy polyester hybrid powdercoat Sample 2
Epoxy powdercoat
Epoxy putty (cured)
Epoxy resin
Epoxy resin - Hardened
Epoxy resin cured
Ethylene/Propylene Rubber
EthyleneTetrafluoroethylene, ETFE
Eyeliner, liquid
Fiberboard
Fiberboard (with DOP)
Fiberboard (with DOP)
Fiberboard (with wax)
Fiberglass resin 1
Fiberglass resin 2
Film (PE and PET)
Filter, Cigarette -cellulose acetate fibers
Filter, cigarette with triacetin
Finger oil
flax fiber
flax wool blend
Floor adhesive (SBR)
Fluoroalkyl acrylate
Fly ash
Gelatin
Glucose
Glue (Bone)
Glue (Fish)
Glue (Hide)
Glue (hide, solid)
Glue (hot-melt)
Glue stick, permanent
Glue stick, temporary
Gum base
Hair gel
Hair gel - volumizing
Hair, human Sample 1
Hair, human Sample 2
Handcream
hemp fiber
hemp wool blend
High impact polystyrene
Hoof, horse
Humic acid
Ink ball point Sample 1
Ink ball point Sample 2
Ink from ink jet printer
Ink, printing
Irgastab (antioxidant)
Isobutylene/acrylonitrile
Kalrez
Kapton Tape
Kapton (Poly-oxydiphenylene-pyromellitimide)
Kerogen 1
Kerogen 2 – from source rock
Kevlar
Kraton 1107
Kraton 1161 PT
Latex Paint
Lignin
Lignosulfonate
Lip balm - Chapstick
Lipstick, all natural
Lipstick, frosted - Lancome
Lipstick, pink
Lowilite 62 (antioxidant)
Lubricant (grease) – Super Lube
Lubricant (Stick) – Door Ease
Make up, eyeliner - liquid
Mascara

Mascara, waterproof
Mascara, with wax Sample 1
Mascara, with wax Sample 2
Mascare, waterproof- with methyl methacrylate, butyl acrylate
Melanin
MMA, Styrene, BA, 2-EHA, 2-EHMA
Moisturizing cream
Motor oil – 10W-30 Mobil
Motor oil – 10W-30 Pennzoil
Motor oil (Non-detergent)
Motor oil (Synthetic)
Mucilage
Nail polish, red
Nail polish, red iridescent
Natural Bristle
nettle fiber
nettle wool blend
Nitrile rubber (glove)
Nitrile Rubber (With DOP)
Norsorex (Poly(noroborene))
Nylon 11
Nylon 12
Nylon 6
Nylon 6/10
Nylon 6/12
Nylon 6/6
Nylon 6/9
Nylon 6T
Oil (Petroleum, crude)
Oil from shale
Oil paint yellow – Windsor Lemon yellow artist oil paint
Olive stone
Packaging, clear with phthalate
Packing film (PE and Nylon 6)
Paint (Styrene, acrylic, plasticizers)
Paint latex
Paint, alkyd
Paint, automotive, clear coat - BASF
Paint, automotive, clear coat - PPG
Paint, automotive, whole – 1995 Sebring Silver
Paint, beverage can
Paint, latex
Paint, spray, black - Rustoleum
PAN Fiber
Paper (Brown)
Paper with printing ink
Paper, coated, glossy
Paper, white
Paper, white, with toner – laser jet toner, polystyrene
Paper, with adhesive – Press-Apply removable label
Paper, yellow, with adhesive – Temporary, universal note
Paperboard
Paraffin wax
Parafilm
Pectin
PEEK Sample 1
PEEK Sample 2
PET (Polyethylene Terephthalate)
PHBV Polyhydroxy butyrate co-valerate
Phenol formaldehyde resin 1
Phenolformaldehyde resin 2
Phenolic resin 1
Phenolic resin 2
Phenolic resin 3
Phenolic resin 4
Photocopy toner (Color) - Cyan 1
Photocopy toner (Color) - Cyan 2
Photocopy toner (Color) - Cyan 3
Photocopy toner (Color) - Cyan 4
Photocopy toner (Color) - Cyan, Styrene Acrylic
Piccolyte A115 (Poly-a-Pinene)
Piccolyte C115 (Polylimonene)
plastic suction cup ball toy EGA
PMMA/BA
Poly 1-butene 1
Poly 1-butene 2
Poly 2-ethyl hexyl acrylate
Poly 4-methyl-1-pentene
Poly acrylamide
Poly acrylic acid/maleic acid sodium
Poly acrylonitrile
Poly allylamine
Poly butyl acrylate
Poly butyl acrylate/acrylic acid/methyl methacrylate
Poly butylene terephthalate
Poly butylmethacrylate with MAA MMA and 2-EHA
Poly butylmethacrylate with MMA and MAA
Poly Chloro Trifluoro Ethylene
Poly D L Lactide
Poly epichlorohydrin
Poly ether sulfone
Poly ethyl acrylate
Poly ethyl acrylate ethyl methacrylate
Poly ethylene glycol
Poly ethylene glycol methacrylate
Poly Ethylene Vinyl Acetate (25% VA)
Poly Ethylene Vinyl Acetate (33% VA)
Poly ethylene vinyl acetate wax blend
Poly Ethylene/Vinyl Acetate

Poly glycolic acid
Poly glycolide
Poly isobutyl methacrylate
Poly isobutyl methacrylate with methacrylic acid
Poly lactic acid
Poly lactide glycolide
Poly lauryl methacrylate
Poly methyl acrylate
Poly methylmethacrylate/butyl acrylate
Poly octadecyl acrylate
Poly vinyl acetate
Poly vinyl chloride/vinyl acetate
Poly vinyl fluoride
Poly vinyl formal
Poly vinyl pyrolidone
Poly vinyl stearate
Poly vinyl toluene
Poly vinylchloride/vinylidinechloride
Poly vinylidene fluoride
Poly α–methylstyrene
Poly(4-tert-butylstyrene)
Poly(styrene-co-methyl methacrylate) styrene 40 mol %, 100µg 700°C
Poly(styrene-co-methyl methacrylate) styrene 40 mol %, 10µg 800°C
Poly(vinyl alcohol-co-ethylene) 32 mol% ethylene
Poly(vinylidine fluoride-co-hexafluoropropylene)
poly-3-hydroxybutyric acid
Polyacetal
Polyacrylic acid
Polyacrylonitrile fiber
Polyacrylonitrile/butadiene/styrene
Polybutylacrylate/butylmethacrylate with diisocyanate
Polybutylmethacrylate 1
Polycaprolactone
Polycarbonate
Polycarbonate – Lexan
Polycarbonate (CD)
Polycarbonate (Lexan)
Polycarbonate film
Polycarbonate with brominated flame retardant
Polycarbonate, with siloxane
Polychloroprene
Polychloroprene 700 after 300
Polydimethylsiloxane
Polyester clear coat with styrene
Polyester clear coating
Polyester powdercoat 1
Polyester powdercoat 2
Polyester resin 1
Polyester resin 2
Polyester resin 3
Polyester resin 4
Polyester resin with methacrylate
Polyester thread
Polyester/epoxy composite
Polyethylene
Polyethylene imine
Polyethylene naphthalate
Polyethylene oxide
Polyethylene oxide/propylene oxide 1
Polyethylene oxide/propylene oxide 2
Polyethylene oxide/propylene oxide 3
Polyethylene styrene vinyl acetate
Polyethylene terephthalate
Polyethylene, high density (HDPE)
Polyethylene, LDPE
Polyethylene, LLDPE
Polyethylmethacrylate
Polyglycolide
Polyimide
Polyisobutyl methacrylate
Polyisobutylene 1
Polyisobutylene 2
Polyisoprene 1
Polyisoprene 2
Polylactide
Polymethylmethacryalte with styrene/BA/EA
Polymethylmethacrylate
Polymethylmethacrylate/butyl acrylate
Polymethyltrifluoropropylsiloxane
Polypropylene
polypropylene film EGA
Polypropylene, atactic
Polypropylene, carbonate
Polypropylene, chlorinated
Polystyrene
Polystyrene (28%)/butadiene (72%)
Polystyrene (70%)/acrylonitrile (30%)
Polystyrene (85%)/butadiene (15%)
Polystyrene acrylonitrile methyl methacrylate
Polystyrene acrylonitrile Methyl methacrylate
Polystyrene acrylonitrile MMA
Polystyrene butyl acrylate
Polystyrene butyl acrylate butyl methacrylate
Polystyrene/ Butadiene (SBS)
Polystyrene/ ethylene-butylene
Polystyrene/acrylonitrile
Polystyrene/acrylonitrile/2-ethylhexyl acrylate
Polystyrene/acrylonitrile/MMA/BA/BMA

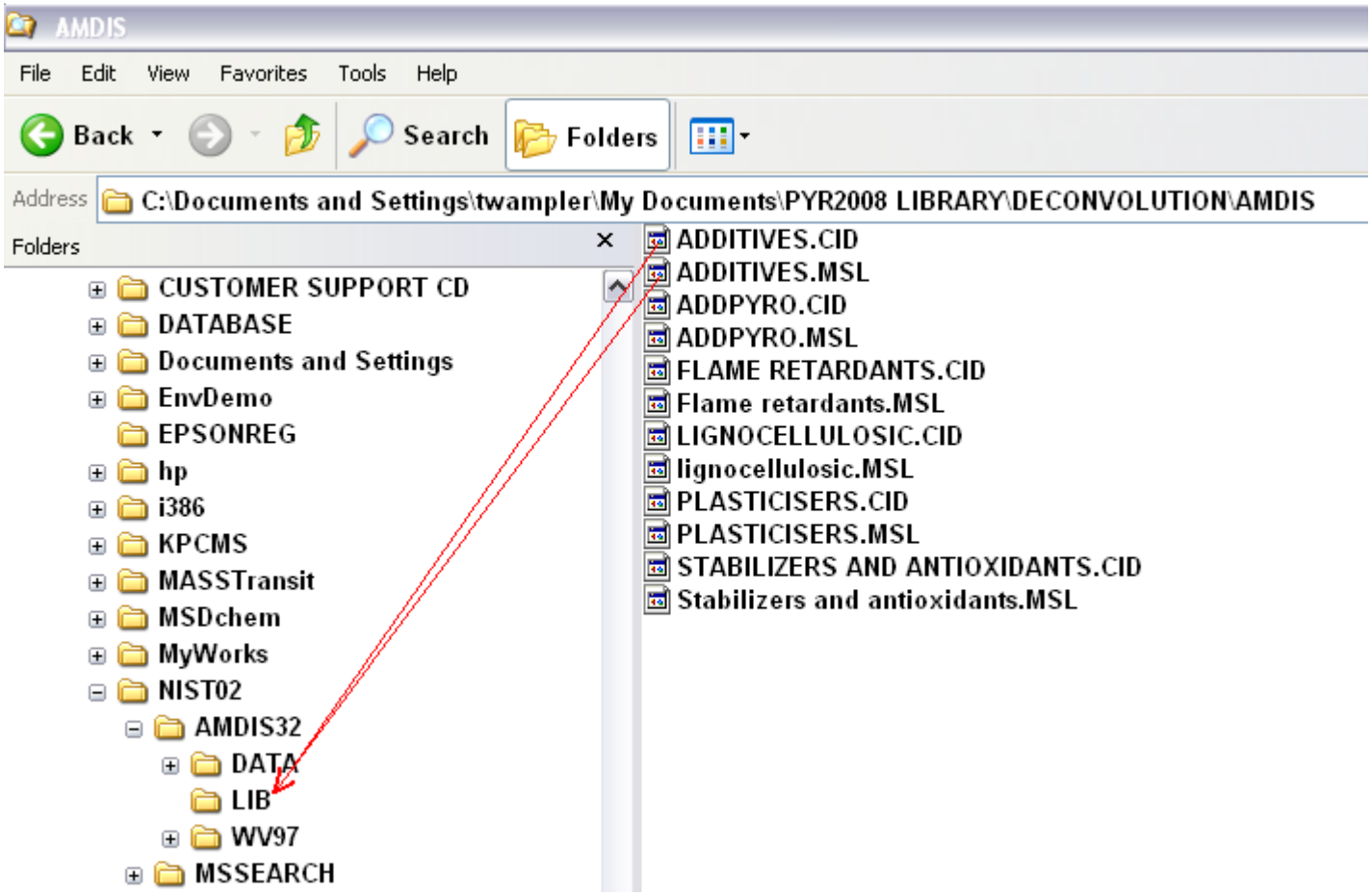
Polystyrene/Butadiene/MMA
Polystyrene/Butadiene/MMA/BA
Polystyrene/ethylene/butylene
Polystyrene/isobutyl methacrylate/2-ethylhexyl acrylate
Polystyrene/methylstyrene
Polystyrene/MMA/2-ethylhexyl acrylate
Polystyrene/MMA/Acrylonitrile
Polystyrene/MMA/BA/BMA
Polystyrene/MMA/BA/BMA/Acrylonitrile
Polystyrene/olefin
Polystyrene/vinyl alcohol
Polyterpene resin
Polyurethane
Polyurethane - Spandex
Polyurethane (Estane)
Polyurethane (Hexane diisocyanate)
Polyurethane (polyester)
Polyurethane (polyether)
Polyurethane (TDI and Butanediol)
Polyurethane (TDI)
Polyurethane (with phthalate)
Polyurethane dispersion
Polyurethane finish – Gloss, clear
Polyurethane foam
Polyurethane foam with triphenyl phosphoric acid
Polyurethane paint – Alkyd with TDI
Polyurethane varnish (TDI)
Polyurethane with styrene, MMA, BA
Polyurethane, oil modified
Polyvinyl alcohol
Polyvinyl butyral, 600°
Polyvinyl chloride
Polyvinylchloride/vinylacetate
Polyvinylidine chloride
Polyvinylpyrrolidone PVP
Porkhide Chew Toy, Smoked, with Terephthalate
PU foam (rigid, packing)
PU foam with styrene and phosphates
PVC (heavily plasticized)
PVC with bis-2-ethylhexylphthalate
PVC with plasticizers
PVC, no plasticizers
PVC/Styrene/MMA
PVC/Styrene/MMA -Clear plastic PVC with poly styrene and poly methyl methacrylate
Rayon
Red artist oil paint – Grumbacher red
Red children's paint - Crayola
Red pigment (PR122)
red plastic (polypropylene) cap EGA
Register Tape 600°C
Resin (Styrene, 2-EHA)
Rubber (Natural)
rubber 85:15 butyl:natural
Rubber bulb (red)
Rubber cement
Rubber, Ethylene (40.1%)/ Propylene
Rubber, Ethylene (54.2%)/ Propylene
Rubber, Ethylene (58.6%)/ Propylene
Rubber, Ethylene (66.8%)/ Propylene
Rubber, Ethylene (77.5%)/ Propylene
Rubber, Ethylene (78.6%)/ Propylene
Rubber, foam, blue (urethane)
Rubber, tire butadiene isoprene styrene
Rubber, tire butadiene, isoprene
Rubber, tire with antioxidant 1
Rubber, tire with antioxidant 2
Saran
Sawdust
Saytex 8010
Shampoo
Shampoo – volumizing shampoo
Shellac (Orange)
Silicone caulk
Silicone rubber 1
Silicone rubber 2
Silicone rubber 3
Silk thread
Sizing, paper, (AKD) – Alkyl ketene dimer
Sizing, paper, (ASA)
Spandex
Spermaceti wax
Styrene Butadiene rubber
Styrene Butadiene rubber - multipurpose
Styrene butylacrylate
Styrene/Butadiene/Isoprene rubber
Styrene/butylacrylate/α-methylstyrene – Food package coating
Styrene/butylmethacrylate/isobutyl methacrylate
Styrene/isoprene rubber
Sucrose
Suede with a phthalate
Sulfonic acid – Aromatic mixture
Sulfonic acid, alkyl – alkyl mix
Sumac EGA 100C per min 100 to 800
Sunblock, SPF 40
Sunscreen, SPF 15
Tape (clear)
Tape, brown mailing – with adhesive, PP film
Tape, clear – Cellulose acetate with phthalate plasticiser

Terpene resin 2
Tetrabromo bisphenol A
Tetrafluoroethylene-hexafluoropropylene copolymer, FEP
Thread, Black, Cotton
Thread, Black, Polyester - PET
Thread, carpet – Nylon 6/6
Thread, Cotton
Thread, Cotton/Polyester
Tinuvin 622 (antioxidant)
Tire Inner tread
Tire main tread 1
Tire main tread 2
Tire Rubber
Tire Rubber (SBI)
Tire Rubber (Sty/But/Acrylonitrile)
Tobacco
Tobacco, menthol
TofuTech Soy Fiber
Tone IX 2300
Toner (photocopy) – Canon NP115
Toner (photocopy) – Mita DC131
Toner (photocopy) – Pitney Bowes 8900
Toner (photocopy) – Savin brand (Styrene/butyl acrylate)
Toner (photocopy) – Styrene, Butyl Acrylate, 2-ethyl hexyl acrylate
Toner (photocopy) – Styrene/Butyl acrylate
Toner (photocopy) – Xerox 1012
Toner (photocopy) – Xerox 2830
Toner (photocopy) – Xerox 9500
Toner (photocopy) –Styrene/Butyl Acrylate/ Butyl Methacrylate
Toner HB 1
Toner KM 2300
Toner PE 733
Toner X 501
Toner XK 1
Tung oil
Tung Oil Finish – Minwax, dried
Tung Oil Finish – Zar, Dried
Tygon tubing
Urea formaldehyde
Urethane acrylic (HDI and Isobornyl acrylate)
Urethane elastomer
Urethane finish
Urethane foam with polystyrene
Urethane foam with polystyrene- dichloropropanol phosphate
Urethane polyester powdercoat
Urethane acrylic (HDI and Isobornyl acrylate)
Urethane elastomer
Urethane finish
Urethane foam with polystyrene
Urethane foam with polystyrene- dichloropropanol phosphate
Urethane polyester powdercoat
Urethane rubber (MDI)
Urethane with BMA and Pyrrolidinone
Urethane with MMA, Styrene, BA, BMA
Varnish (Spray, clear)
Vectran LCP (liquid crystal polymer)
vinyl film EGA
Vinyl siding
Vinyl with benzyl butyl phthalate
Viton
Water color (red, solid)
Water color red – Cotman cadium red
Water color yellow – Cotman cadmium yellow pale
Wax, petroleum
White acrylic artist color – Liquitex iridescent white
White acrylic paint
White oil pastel
Wood (pine)
Wood, Aproomosia
Wood, Iroko
Wool
Yellow Pigment 13

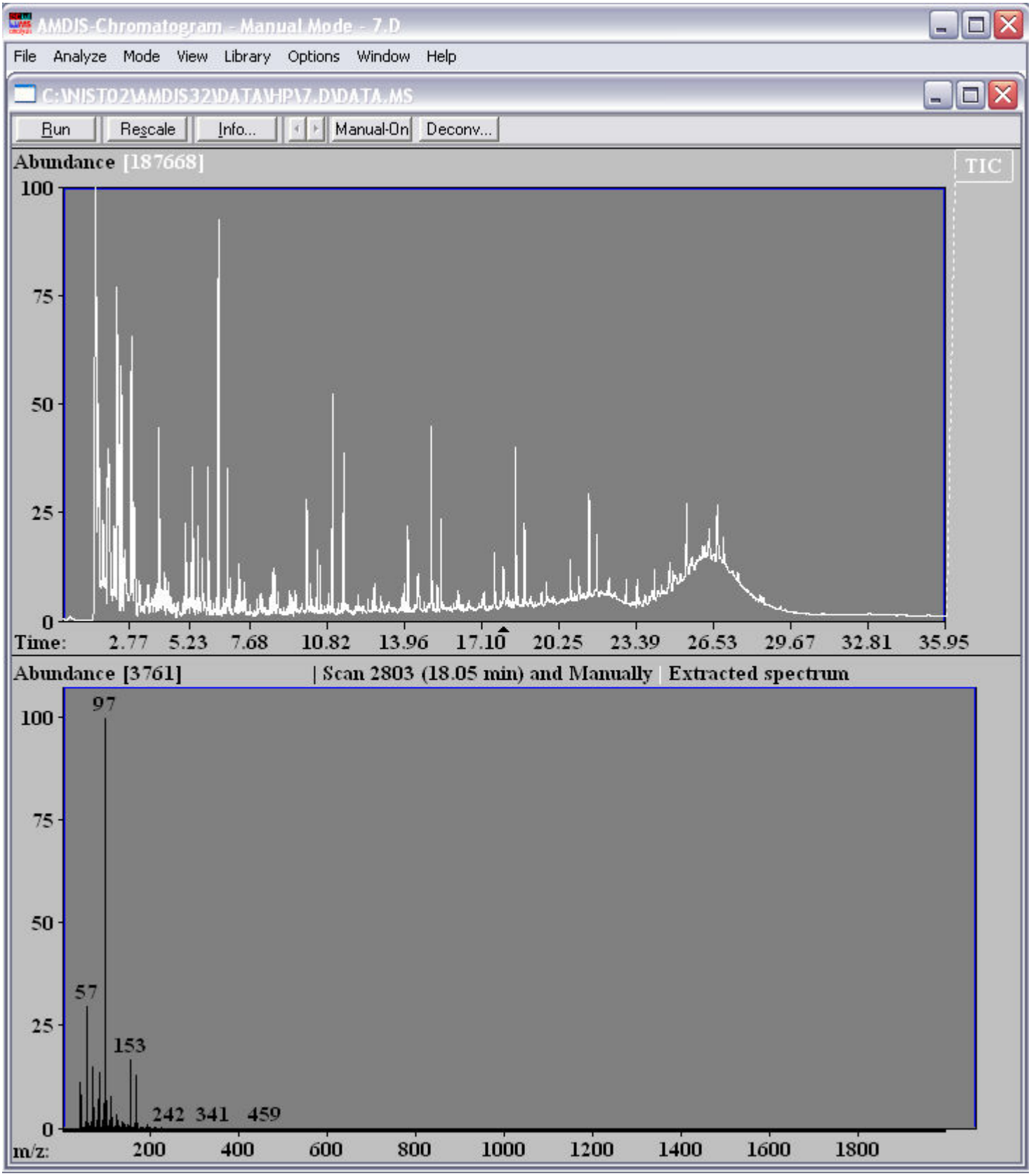
DECONVOLUTION USING AMDIS

Most GCs now come with AMDIS software already loaded on the computer. If you do not have a copy, the AMDIS software is available for download from www.amdis.net. After loading the software, you must add the CDS libraries (Additives, Plasticisers, Pyrolysis products, etc.) from the CDS Library CD to the Nist AMDIS folder on your computer.

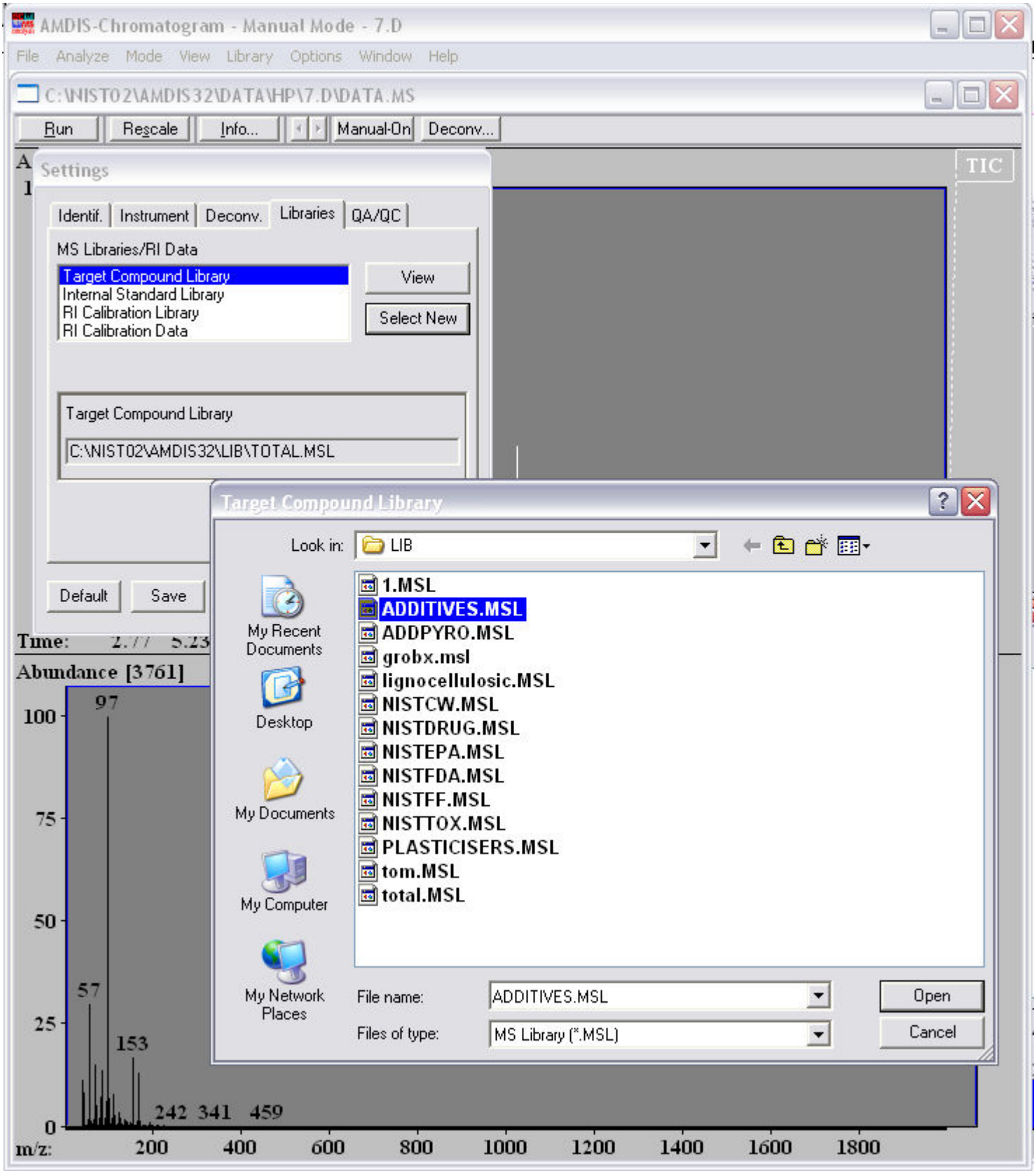
A library has two components, one with the extension .msl and the other with the same name, but the extension cid. You need both, for example, ADDITIVES.CID AND ADDITIVES.MSL to perform searches. These files must be added to the NIST AMDIS LIB folder on your computer from the AMDIS folder on the CDS Library CD.



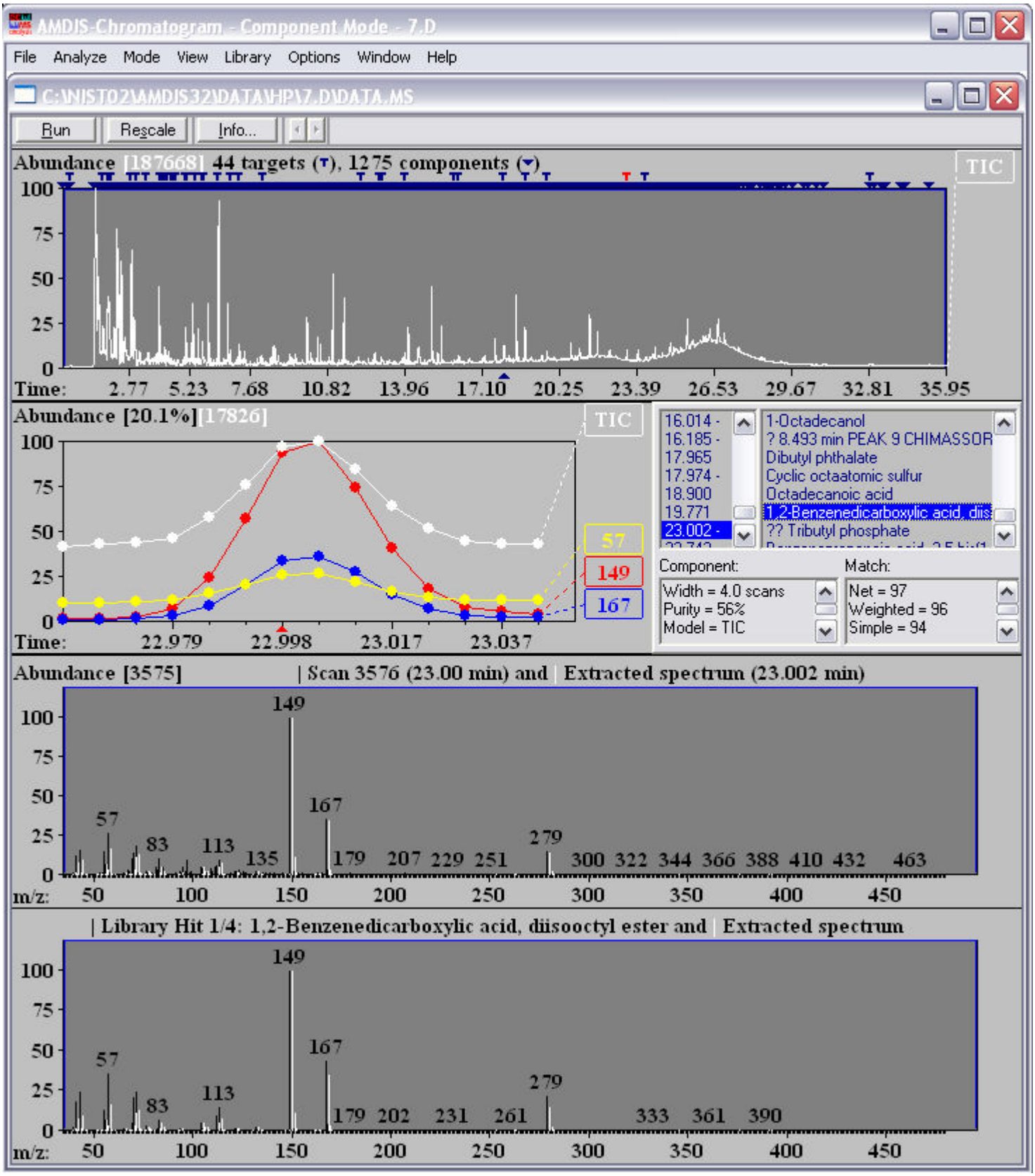
Open a chromatogram by selecting FILE then OPEN. To deconvolute using the current library, just press RUN.



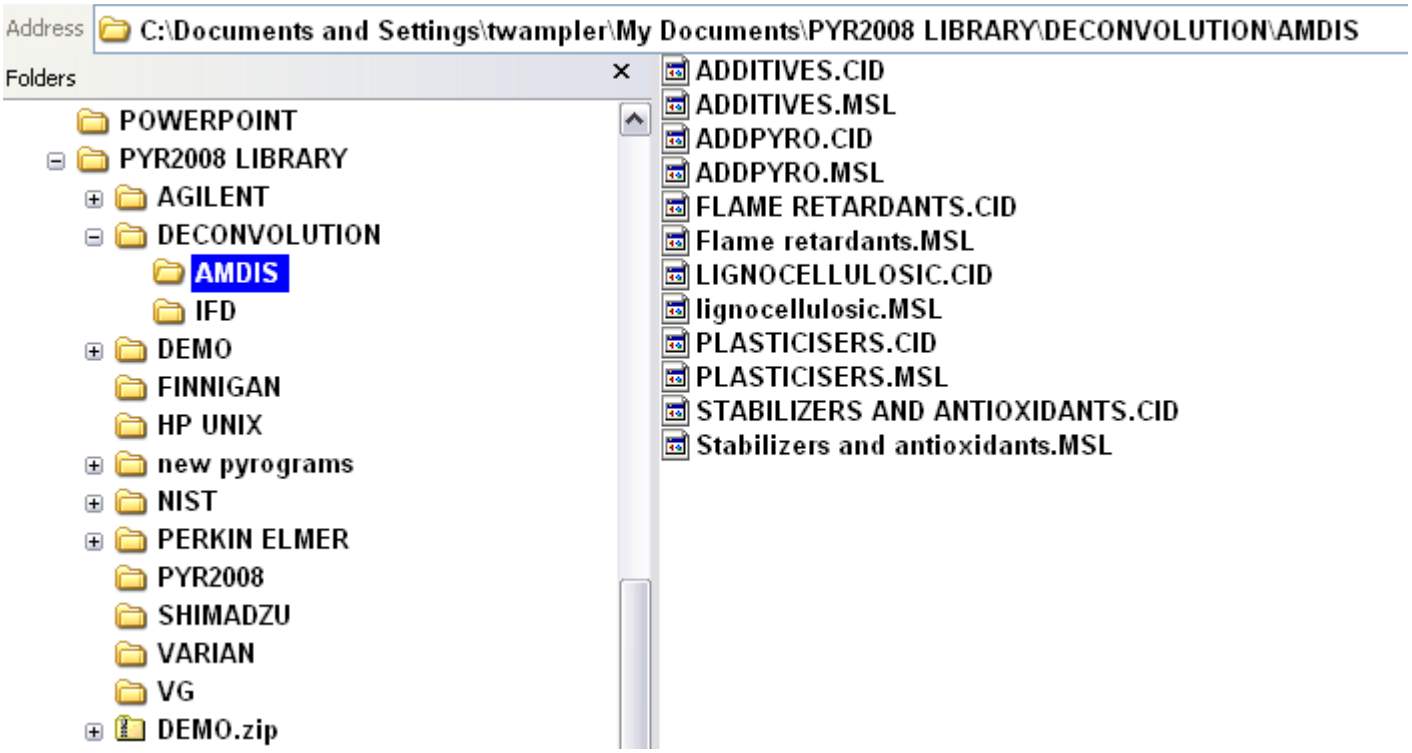
To select another library, go to ANALYZE, then SETTINGS, LIBRARIES and SELECT NEW to select the desired library for searching. After selecting the library, press SAVE on the Settings window and the software will reanalyze the chromatogram with the new library.



After deconvoluting the chromatogram, target compounds (in the library) are marked with a T above the chromatogram. Clicking on a T will show the spectrum of that peak, plus the library spectrum and name of the compound in the library. In this case, a phthalate plasticiser has been identified at 23 minutes. Also, clicking on the compound name in the box (right, center) will indicate the peak by turning the T red for that compound.



The AMDIS folder in the CDS Library contains various libraries and sub-libraries. The ADDITIVES library contains spectra for over 260 individual compounds and the ADDPYRO library contains over 100 spectra for compounds made by pyrolyzing additives. The FLAME RETARDANTS, PLASTICISERS and STABILIZERS libraries are specific sub-libraries of the larger ADDITIVES library. The LIGNOCELLULOSIC library is a separate library of over 200 compounds found in the pyrograms of lignin and cellulose, that is, from biomass and biofuels materials like wood, grass, straw, switchgrass and so on. Taken together, the AMDIS libraries contain over 550 spectra. The compounds found in the ADDITIVES and LIGNOCELLULOSIC libraries are listed on the following pages.



ADDITIVE LIBRARY contents

1,4-Benzenediamine, N-(1,3-dimethylbutyl)-N'-phenyl-
2-Mercaptobenzimidazole
2-Mercaptobenzothiazole
2-Propenoic acid, 2-methyl-, 2-(dimethylamino)ethyl ester
Benzenecarboperoxoic acid, 1,1-dimethylethyl ester
Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, thiodi-2,1-ethanediyl ester, thiodi-2,1-ethanediyl ester
Di-tert-butyl peroxide
Hexanoic acid, 2-ethyl-, 1,2-ethanediylbis(oxy-2,1-ethanediyl) esterl) ester
Methanone, bis[4-(dimethylamino)phenyl]-
Phthalic acid, bis(7-methyloctyl) ester
Propanoic acid, 3,3'-thiobis-, didodecyl ester
tert-Butyl Hydroperoxide
tri(2-Ethylhexyl) trimellitate
(Z)-9-Octadecenoic acid butyl ester
1,1 Dichloroethane
1,1,1trichloroethane
1,1,2,3,4,4 Hexachlorobutadiene
1,2,4-Benzenetricarboxylic acid, trihexyl ester
1,2,5,6,9,10-Hexabromocyclododecane
1,2-Dichloroethylene
1,3,5-triazine-2,4,6 triamine
1,3,5-Trimethyl-2,4,6-tris(3,5-di-tert-butyl-4-hydroxybenzyl)-benzene)-benzene
1,3-propanediol, 2-ethyl-2-(hyroxymethyl)-
12-hydroxy stearic acid
1-Hexadecanol
1-octadecanol
1-Propanol, 2,3-dichloro-, phosphate (3:1)
2 ethyl hexyl epoxystearate
2,2,4,4,5,5-Hexabromobiphenyl
2,2,4,4,6,6-Hexabromobiphenyl
2,2,4,5,5-Pentabromobiphenyl
2,2,4,5,6-Pentabromobiphenyl
2,2,4,5-Tetrabromobiphenyl
2,2,4-Trimethyl-1,3-pentanediol diisobutyrate
2,2,5,5,-Tetrabromobiphenyl
2,2,5-Tribromobiphenyl
2,2'-Dihydroxy-1,1-thiodinaphthalene
2,2'-Ethylidenebis(4,6-di-tert-butylphenol)
2,3,5 Tribromobiphenyl
2,4,5-Tribromobiphenyl
2,4,6-Tribromobiphenyl
2,5 di t butyl hydroquinone
2,6 di t butyl hydroquinone
2,6-bis-tertbutyl phenol
2-[(2-ethylhexyl)oxy] ethanol
2-butoxyethyl phthalate
2-ethyl hexy adipate
2-ethyl hexyl tetrabromophthalate (TBPH)
2-ethylhexyl phosphate
2-ethylhexyl sebacate
2-ethylhexyl,-2,3,4,5-tetrabromo benzoate
2-hydroxy-N-1H-1,2,4-triazol-3
2-Mercaptobenzimidazole
2-Methoxyethyl phthalate
2-Nitrophenyl octyl ether
2-phenyl indole
2-Propenoic acid, 2-(dimethylamino)ethyl ester
2-Propenoic acid, 2-methyl-, 2-(diethylamino)ethyl ester
3,3,4,4,5,5-Hexabromobiphenyl
3,3,5,5-Tetrabromobiphenyl
4,4'-Azo-bis(4-cyanopentanoic acid)
6 PPD
9H-Thioxanthen-9-one, 2-chloro-
9-Octadecenamide
Acetophenone, 4'-hydroxy-
Advastab 800
Advastab 802
Advawax
Allyl 2,4,6-tribromophenyl ether
Alpha Tocopherol
Anox 20
Anox 330
Anox 70
Anox PP18
Antioxidant 2246
Antioxidant 425
Antioxidant 736
Antioxidant IP
Antioxidant PAN
Aramide E
Azodicarbonamide
Benzamide, 2-hydroxy-N-1H-1,2,4-triazol-3-yl-
Benzene
Benzene sulfonyl hydrazide
Benzene, 1,1'-[1,2-ethanediylbis(oxy)]bis[2,4,6-tribromo-
Benzenepropanoic acid, 3-(1,1-dimethylethyl)-4-hydroxy-5-methyl-, 1,2-ethanediylbis(oxy-2,1-ethanediyl) esterhyl-, 1,2-ethanediylbis(oxy-2,1-ethanediyl) ester

Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, 2-[3-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-oxopropyl] hydrazide, 2-[3-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-oxopropyl]hydrazidepyl]hydrazide

Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester, octadecyl ester

Benzoic Acid, 2,3,4,5-tetrabromo, 2-ethylhexyl ester (TBB)

Benzoic acid, 2-hydroxy-, phenyl ester
Benzophenone
Benzyl butyl phthalate
bis 2ethylhexyl azelate
Bis-octylphenylamine
Bumetrizole
Butadiene
Butanoic acid, 3-oxo- ethyl ester
Butoxyethoxy ethyl adipate
Butoxyethyl adipate
Butoxyethyl butyl Phthalate
Butyl citrate
Butyl Cyclohexyl Phthalate
Butyl Decyl Phthalate
Butyl ethylhyxyl Phthalate
Butyl Isobutyl Phthalate
Butyl Methyl Phthalate
Butyl Methylnonyl Phthalate
Butyl Octyl Phthalate
Butyl oleate
Butyl phthalate butyl glycolat
Butyl stearate
Butylated Hydroxy Anisole
Butylated Hydroxytoluene
Carbon disulfide
Carbon tetrachloride
Chimasorb 90
Chlorobenzene
Chlorotoluene
Cresyl diphenylphosphate
Decanedioic acid, bis(1,2,2,6,6-pentamethyl-4-piperidinyl) esterster
Decanedioic acid, bis(2,2,6,6-tetramethyl-4-piperidinyl) esterer
Decyl acetate
Decyl Octyl Phthalate
Dehydroacetic acid
Di n octyl phthalate
Dibenzal(oxalyl dihydrazide)
Dibenzyl Phthalate
Dibutyl adipate
Dibutyl itaconate
Dibutyl phthalate
Dibutyl sebacate
Dibutyl tartrate
Dibutyl tin dilaurate
Dichlorobenzene
Dichloroethane
Dichloroethene
Dichloropropane
Dichloropropene
Dicyclohexyl phthalate
Didecyl phthalate
Didodecyl Phthalate
Diethyl adipate
Diethyl phthalate
Diethyl sebacate
Diethyl succinate
Diethylene glycol dibenzoate
Diheptyl phthalate
Diisobutyl adipate
Diisobutyl fumarate
Diisobutyl phthalate
Diisodecyl adipate
diisodecyl phthalate
Diisononyl phthalate
Diisooctyl adipate
Diisooctyl phthalate
Diisopropyl ether
Dimethyl adipate
Dimethyl phthalate
Dimethyl sebacate
Dinonyl Phthalate
Dioctadecyl disulfide
Dioctyl phthalate
Dioctyl Terephthalate (DOTP)
Dioxane
Dioxybenzone
Dipentarythrital
Dipentyl Phthalate
Diphenyl phthalate
Diphenyl propanedione
Dipropyl phthalate
Distearyl thiodipropionate
Diundecyl Phthalate
dl-Camphoroquinone
Dodecanamide
Dodecanoic acid, 1,2,3-propane

Ethane diol
Ethanedioic acid, bis[(phenylmethylene)hydrazide]
Ethanone, 1-(4-ethoxyphenyl)-
Ethanone, 2-hydroxy-1,2-bis(4-methoxyphenyl)-
Ethanone, 2-hydroxy-1,2-diphenyl-
Ethoxyethyl Phthalate
Ethyl 4-acetylbutyrate
Ethyl acetate
Ethyl benzene
Ethyl chloride
Ethyl citrate
Ethyl palmitate
Ethylbutyl Phthalate
Ethyleneglycol monosteaarate
Ethylparaben
Fireguard 2000
Glycerine
Glycerol tricaprylate
HALS 1
Hexabromo benzene
Hexabromocyclododecane
Hexyl acetate
Hydroperoxide, 1-methyl-1-phenylethyl
Irganox 1035
Irganox 245
Isopropyl Phthalate
Lowilite 20S
Lowilite 22
Lowilite 24
Lowilite 26
Lowilite 27
Lowilite 28
Lowinox AH25
Lowinox CA22
Lowinox MD24
Lowinox TBM6
Lowinox TBP6
Methanone, (4-hydroxyphenyl)phenyl-
Methanone, (4-methylphenyl)phenyl-
Methanone, [4-(dimethylamino)phenyl]phenyl-
Methanone, bis(2,4-dihydroxyphenyl)-
Methanone, bis(2-hydroxy-4-methoxyphenyl)-
Methanone, bis[4-(diethylamino)phenyl]-
Methyl methacrylate
Methyl ricinoleate
Methylene chloride
methylethylbenzene
Methyloctyl Phthalate
Methylparaben
Methylpentyl Phthalate
MHHPA
MIBK
Naugard 445
N-butyl benzenesulfonamide
NN-diphenylthiourea
Nonanediotic acid dimethyl ester
Nonanediotic acid, dihexyl ester
Nonyl acetate
Octisizer
Octyl acetate
Oxiraneoctanoic acid, 3-octyl-, 2-ethylhexyl ester
Pentabromo toluene
Pentabromophenol
Pentaerythritol
Pentaerythritol tetrakis[3-(3',5'-di-tert-butyl-4'-hydroxyphenyl)propionate]enyl)propionate]
Phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylpropyl)--
Phenol, 2-(5-chloro-2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylethyl)-ylethyl)-
Phenol, 2-methyl-4-(1,1,3,3-tetramethylbutyl)-
Phenol, 4-(2,2,4-trimethylpentyl)-
Phenol, 4,4',4"-(1-methyl-1-propanyl-3-ylidene) tris[2-(1,1-dimethylethyl)-5-methyl-dimethylethyl)-5-methyl-
Phosphoric acid, bis[2-chloro-1-(chloromethyl)ethyl] 2,3-dichloropropyl ester
Phthalic anhydride
Propanenitrile, 2,2'-azobis[2-methyl-
Propanoic acid, 3,3'-thiobis-, ditetradecyl ester
Propylparaben
Santicizer E15
Santicizer M17
Santoflex A
Santowhite
Sorbitol
Stearamide
Stearic acid
Styrene
Trimellitic acid tri-n-butyl ester
tris(1,3-dichloro-d-propyl)phosphate

PYROLYSIS PRODUCTS OF ADDITIVES
Tinuvin 622 – 15 peaks
3,3Dithiopropionic acid – 4 peaks
Lowinox 22m46 – 16 peaks
Irgastab FS042 – 4 peaks
Irganox 3790 – 12 peaks
Anox 20 – 20 peaks
Chimassorb 944 – 20 peaks
Chimassorb 119 – 20 peaks
Saytex 8010 - 3 peaks

LIGNOCELLULOSIC LIBRARY SPECTRA

1,2,3-Trimethoxybenzene
1,2,4-Trimethoxybenzene
1,2-Benzenediol
1,2-Benzenediol, 3-methoxy-
1,2-Benzenediol, 3-methyl-
1,2-Benzenediol, 4-methyl-
1,2-Cyclopentanedione, 3-methyl-
1,3-Benzenediol, 2-methyl-
1,3-Benzenediol, 4-ethyl-
1,3-Cyclohexadiene
1,3-Cyclopentadiene
1,3-Cyclopentanedione, 2-methyl-
1,3-Dioxolane, 2-ethenyl-4-methyl-
1,4-Benzenediol, 2,6-dimethyl-
1,4-Benzenediol, 2-methoxy-
1,4-Benzenediol, 2-methyl-
1,6-Anhydro-á-D-glucofuranose
1,6-Anhydro-á-D-glucopyranose (levoglucosan)
1H-Inden-1-one, 2,3-dihydro-
1H-Indene, 2,3-dihydro-1,2-dimethyl-
1H-Indene, 3-methyl-
1-Hydroxy-2-butanone
1-Penten-3-one
1-Pentyn-3-ol, 3-methyl-
1-Propanol
1-Propene, 2-methyl-
2(3H)-Furanone, 5-ethyldihydro-
2(3H)-Furanone, 5-methyl-
2(3H)-Furanone, dihydro-3-methylene-
2(5H)-Furanone
2(5H)-Furanone, 5-methyl-
2,3-Butanedione
2,3-Dimethylanisole
2,3-Dimethylhydroquinone
2,3-Pentanedione
2,4-Dimethoxyphenol
2,5-Dimethoxy-4-ethylbenzaldehyde
2,5-Dimethylanisole
2',4'-Dihydroxypropiophenone
2-Butanone
2-Butanone, 3-hydroxy-
2-Butenal
2-Butenal
2-Butenal, 2-methyl-
2-Cyclopenten-1-one, 2,3-dimethyl-
2-Cyclopenten-1-one, 2-hydroxy-3-methyl-
2-Cyclopenten-1-one, 2-methyl-
2-Cyclopenten-1-one, 3-methyl2-
2-Furancarboxaldehyde, 5-(hydroxymethyl)-
2-Furancarboxaldehyde, 5-methyl-
2-Furancarboxylic acid
2-Furanmethanol
2H-Pyran, 5,6-dihydro-2-methyl-
2-Methoxy-4-vinylphenol
2-Methoxy-5-methylphenol
2-Methoxy-6-methylphenol
2-Methoxyresorcinol
2-Pentanone
2-Pentenoic acid
2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-
2-Propanone, 1-(acetyloxy)-
2-Propanone, 1-hydroxy-
2-Propenal
2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-
2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-, methyl ester
3,4-Dimethoxy-5-hydroxybenzaldehyde
3,4-Dimethoxytoluene
3,4-Dimethylanisole
3,4-Dimethylbenzyl alcohol
3,5-Dimethoxy-4-hydroxycinnamaldehyde
3,5-Dimethoxy-4-hydroxytoluene

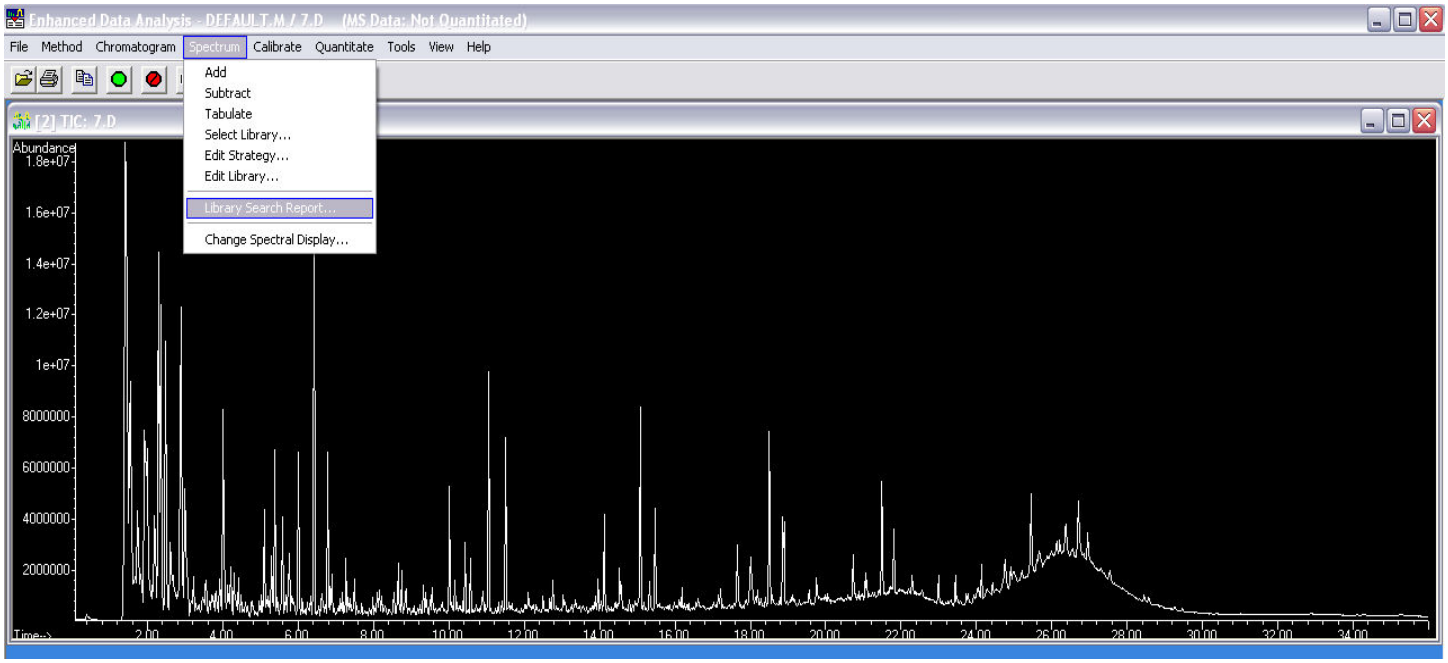
3',5'-Dimethoxyacetophenone
3-Allyl-6-methoxyphenol
3-Allyl-6-methoxyphenyl acetate
3-Furaldehyde
3-Furanmethanol
3-Hydroxy-4-methoxymandelic acid
3-Methoxy-5-methylphenol
3-Pentanone
4-Acetoxy-3-methoxyacetophenone
4H-Pyran-4-one, 3,5-dihydroxy-2-methyl-
4-Hydroxy-2-methoxybenaldehyde
4-Methoxybenzene-1,2-diol
4-Methyl-2,5-dimethoxybenzaldehyde
5-tert-Butylpyrogallol
7-Hydroxy-6-methoxy-2H-1-benzopyran-2-one
Acetaldehyde
Acetaldehyde, hydroxy-
Acetic acid
Acetic acid, methyl ester
Acetophenone, 4'-hydroxy-
Benzaldehyde
Benzaldehyde, 3-hydroxy-
Benzaldehyde, 4-hydroxy-3,5-dimethoxy-
Benzaldehyde, 4-methyl-
Benzene
Benzene, 1,2,3-trimethoxy-5-methyl
Benzene, 1,2,4-trimethoxy-5-(1-propenyl)-, (Z)-
Benzene, 1,2,4-trimethyl-
Benzene, 1,2-dimethoxy-
Benzene, 1,2-dimethoxy-4-(1-propenyl)-
Benzene, 1,3,5-trimethyl-
Benzene, 1,3-dimethyl-
Benzene, 1,4-dimethoxy-2-methyl-
Benzene, 4-ethenyl-1,2-dimethoxy-
Benzene, 5-ethoxy-1,3-bis(hydroxymethyl)-
Benzene, hexamethyl-
Benzeneacetic acid, 4-hydroxy-3-methoxy-, methyl ester
Benzofuran, 2,3-dihydro-
Benzofuran, 2-methyl-
Benzofuran, 7-methyl-
Benzoic Acid
Benzoic acid, 3-hydroxy-
Benzoic acid, 4-formyl-
Benzoic acid, 4-hydroxy-
Benzoic acid, 4-hydroxy-3,5-dimethoxy-
Benzoic acid, 4-hydroxy-3-methoxy-
Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester
Butanal
Carbon dioxide
Cyclopentanol
Cyclopentene-1,4-dione
d-allose
d-arabinose
d-galactose
d-glucose
d-Lyxose
d-mannose
d-Ribose
d-talose
d-xylose
Ethanethiol
Ethanone, 1-(2-furanyl)-
Ethanone, 1-(2-hydroxy-4,6-dimethoxyphenyl)-
Ethanone, 1-(3,4-dimethoxyphenyl)-
Ethanone, 1-(3-hydroxy-4-methoxyphenyl)-
Ethanone, 1-(3-methoxyphenyl)-
Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-
Ethanone, 1-(4-hydroxy-3-methoxyphenyl)-
Eugenol
Formaldehyde
Furan
Furan, 2,4-dimethyl-
Furan, 2,5-dihydro-
Furan, 2,5-dimethyl-
Furan, 2-ethyl-5-methyl-
Furan, 2-methyl-
Furan, 2-propyl-
Furan, 3-methyl-
Furfural
Hydroquinone
Indene
Isomaltol
Isopropyl Alcohol
Ketene
l-arabinose
Limonene
L-Lyxose
l-mannose
Maltol
Mequinol
Methane, chloroo-
Phenol
Phenol, 2,3-dimethyl-
Phenol, 2,4-dimethyl-
Phenol, 2,5-dimethyl-
Phenol, 2,6-dimethoxy-
Phenol, 2,6-dimethoxy-4-(2-propenyl)-
Phenol, 2,6-dimethyl-
Phenol, 2-ethyl-

Phenol, 2-ethyl-4-methyl-
Phenol, 2-ethyl-5-methyl-
Phenol, 2-ethyl-6-methyl-
Phenol, 2-methoxy-
Phenol, 2-methoxy-3-(2-propenyl)-
Phenol, 2-methoxy-3-methyl-
Phenol, 2-methoxy-4-(1-propenyl)-
Phenol, 2-methoxy-4-(1-propenyl)-, (E)-
Phenol, 2-methoxy-4-(1-propenyl)-, (Z)-
Phenol, 2-methoxy-4-methyl-
Phenol, 2-methoxy-6-(1-propenyl)-
Phenol, 2-methyl-
Phenol, 3,4-dimethoxy-
Phenol, 3,4-dimethoxy-, acetate
Phenol, 3,4-dimethyl-
Phenol, 3,5-dimethyl-
Phenol, 3-ethyl-
Phenol, 3-methoxy-2-methyl-
Phenol, 3-methyl-
Phenol, 4-ethyl-
Phenol, 4-ethyl-2-methoxy-
Phenol, 4-ethyl-2-methyl-
Phenol, 4-methoxy-3-methyl-
Phenol, 4-methyl-
Propanal, 2,3-dihydroxy-
Propanoic acid, 2-oxo-, methyl ester
Propene
p-Xylene
Resorcinol
Salicylic Acid
Styrene
Toluene
Vanillin
Vinylfuran
Xylene

AUTOMATIC LIBRARY SEARCHING USING AGILENT CHEMSTATION

AGILENT LIBRARY SEARCH REPORT

In Agilent Chemstation Enhanced Data Analysis, under SPECTRUM is the option “Library Search Report...”. When this is selected, Chemstation searches the spectra in the chromatogram against the spectra in a selected library to find matches.



The results of the search may be printed, or just displayed to the screen, and give the retention time, name of the matching compound or compounds in the library and the quality of the match. In this example, a phthalate plasticiser has been identified at 23 minutes.