“Investigation of Low-Reactivity Solvents”

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Final Report Presented by

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“Investigation of Low-Reactivity Solvents”

Project Objectives

- Produce database of physical and chemical properties for selected solvents and solvent mixtures

- Develop detailed chemical speciation for selected hydrocarbon solvents

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Database Solvent Parameters

Properties	Basis for Selection; notes
Name, trade name, synonyms	Allows lookup by a number of naming systems
CAS number	Unique reference number; useful for links to other databases
Formula, molecular weight	Provides basic chemical information; not applicable for mixtures
Structure	Shows graphical structure; not applicable for mixtures
Chemical Class	Allows comparison with other chemically related substances
MP, BP	Provides information for storage/shipping conditions
Vapor pressure (at reference temperature)	Gives an estimate of volatility
Evaporation rate (relative to butyl acetate)	A practical measure of volatility
Flash point	Significant for safe handling
Specific Gravity	Allows conversion between mass and volume
Viscosity	Provides an insight into pouring/mixing characteristics
Henry's law constant	Describes partitioning from aqueous phase into vapor
Solubility in water	Important for formulation compatibility and disposal
Log K_{ow}	Gives info about partitioning between aqueous environment and biomass
Kauri-butanol number	Not applicable for all solvent classes
Hildebrand parameter	Widely used to allow comparisons of solvency abilities
k_{OH}	Rate constant with hydroxyl radical, a scavenger for atmospheric VOCs
MIR	A measure of photochemical reactivity
Toxic Air Contaminant	Compliance with current regulations

"Investigation of Low-Reactivity Solvents"

Database Solvent Selection

- Began with list of 383 solvents from ARB Consumer Product Survey
- Identified some duplicate names
- Obtained CAS numbers;
  sorted to reveal duplicate names/CAS number assignments
- Prepared ranked list of top 100 solvents, by sales volumes
- Draft list presented to ARB and RRAC
  for comments, additions, deletions

“Investigation of Low-Reactivity Solvents”

List of Solvent Classes

- Alcohols (ALC)
- Esters (EST)
- Glycols (GLY)
- Glycol Ethers (GLYE)
- Halogenated (HAL)
- Hydrocarbons (HYD)
- Ketones (KET)
- Nitrogen-Containing (NIT)
- Propellants (PROP)
- Miscellaneous (MISC)

"Investigation of Low-Reactivity Solvents"

Members of Solvent Classes

Alcohols
1-butanol
1-propanol
2-butanol
2-ethyl-1-hexanol
2-methyl-2-propanol
2-propanol
benzyl alcohol
cyclohexanol
ethanol
isobutanol
methanol

Esters
2-butoxyethyl acetate
2-ethoxyethyl acetate
2-methoxyethyl acetate
butyl acetate
dimethyl adipate
dimethyl glutarate
dimethyl succinate
dipropylene glycol methyl ether acetate
ethyl acetate
ethyl-3-ethoxypropionate
glyceryl triacetate
isobutyl acetate
isobutyl isobuytrate
isopentyl acetate
isopropyl acetate
methyl acetate
n-amyl acetate
n-propyl acetate
propylene glycol ethyl ether acetate
propylene glycol methyl ether acetate
t-butyl acetate

Glycols
2-methyl-2,4-pentanediol
diethylene glycol
dipropylene glycol
ethylene glycol
propylene glycol

Glycol Ethers
1-methoxy-2-propanol
2-butoxyethanol
diethylene glycol monoethyl ether
diethylene glycol monomethyl ether
diethylene glycol mono-n-butyl ether
dipropylene glycol methyl ether
dipropylene glycol mono butyl ether
dipropylene glycol n-butyl ether
propylene glycol monobutyl ether
propylene glycol mono-t-butyl ether
propylene glycol n-propyl ether

Halogenated
1,1,1-trichloroethane
1,1,2-trichloroethylene
1,4-dichlorobenzene
chlorobenzene
methylene chloride
monochlorotoluene
parachlorobenzotrifluoride

Nitrogenous
2-amino-2-methyl-1-propanol
diethanolamine
ethanolamine
N-methylpyrrolidone
triethylamine

Ketones
acetone
cyclohexanone
diacetone alcohol
diisobutyl ketone
isophorone
methyl amyl ketone
methyl ethyl ketone
methyl isoamyl ketone
methyl isobutyl ketone
methyl isopropyl ketone
methyl propyl ketone

Miscellaneous
2-cyano-2-propenoic acid, ethyl ester
acetic acid
acrolein
decamethylcyclopentasiloxane
decamethyltetrasiloxane
dodecamethylcyclohexasiloxane
dodecamethylpentasiloxane
hexamethylcyclotrisiloxane
hexamethyldisiloxane
methyltrimethoxysilane
methyltris(trimethylsiloxy)silane
octamethylcyclotetrasiloxane
octamethyltrisiloxane
pentane-1,5-dial
tetrahydrofuran
tetrakis(trimethylsiloxy)silane

Propellants
1,1,1,2-tetrafluoroethane
1,1-difluoroethane
butane
dimethyl ether
isobutane
propane

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Members of Hydrocarbon Solvent Class

aliphatic distillate	64742525
C9-11 Isoparaffin	68551166
diesel fuel	68334305
heavy aliphatic solvent naphtha	64742967
heavy alkylate solvent naphtha	64741657
hydrofinished solvent refined parafinic petroleum oil	64742547
hydrotreated light distillate	64742478
hydrotreated light naphtha	64742490
hydrotreated heavy naphtha	64742489
isomeric hexanes	73513425
isoparaffinic solvent	64741668
kerosene	8008206
lactol spirits	64741555
medium aliphatic solvent naphtha	64742887
methylhexanes	25495889
mineral oil	8012951
mineral spirits	64742887
naphtha (light)	64741840
odorless mineral spirits	64742478
petroleum distillate	64742014
severely hydrotreated middle distillate oil	64742467
Stoddard solvent	8052413
VM&P naphtha	64742898
aromatic hydrocarbon	68410162
light aromatic solvent naphtha	25551137
heavy aromatic solvent naphtha	64742945
xylenes	1330207

CAS number sorted

xylenes	1330207
kerosene	8008206
mineral oil	8012951
Stoddard solvent	8052413
methylhexanes	25495889
light aromatic solvent naphtha	25551137
lactol spirits	64741555
heavy alkylate solvent naphtha	64741657
isoparaffinic solvent	64741668
naphtha (light)	64741840
petroleum distillate	64742014
severely hydrotreated middle distillate oil	64742467
hydrotreated light distillate	64742478
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hydrotreated light naphtha	64742490
aliphatic distillate	64742525
hydrofinished solvent refined parafinic petroleum oil	64742547
medium aliphatic solvent naphtha	64742887
mineral spirits	64742887
VM&P naphtha	64742898
heavy aromatic solvent naphtha	64742945
heavy aliphatic solvent naphtha	64742967
diesel fuel	68334305
aromatic hydrocarbon	68410162
C9-11 Isoparaffin	68551166
isomeric hexanes	73513425

"Investigation of Low-Reactivity Solvents"

Members of Hydrocarbon Solvent Class

Hydrocarbons	
Aromatic 100	Mineral Spirits, Type IA
Aromatic 150	Mineral Spirits, Type IB
cyclohexane	Mineral Spirits, Type IC
diesel Fuel #2	Mineral Spirits, Type IIA
d-limonene	Mineral Spirits, Type IIB
ethylbenzene	Mineral Spirits, Type IIC
heptane	Mineral Spirits, Type IIIC
heptanes	Mineral Spirits, Type IVA
hexane	Mineral Spirits, Type IVB
hexanes	Mineral Spirits, Type IVC
kerosene	ortho-Xylene
lactol spirits	para-Xylene
meta-xylene	Pine oil
methylcyclohexane	toluene
methylcyclopentane	VM&P Naptha, Type I
mineral oil	VM&P Naptha, Type II
	VM&P Naptha, Type III
	VM&P Naptha, Type IV
	Xylenes (Mixture)

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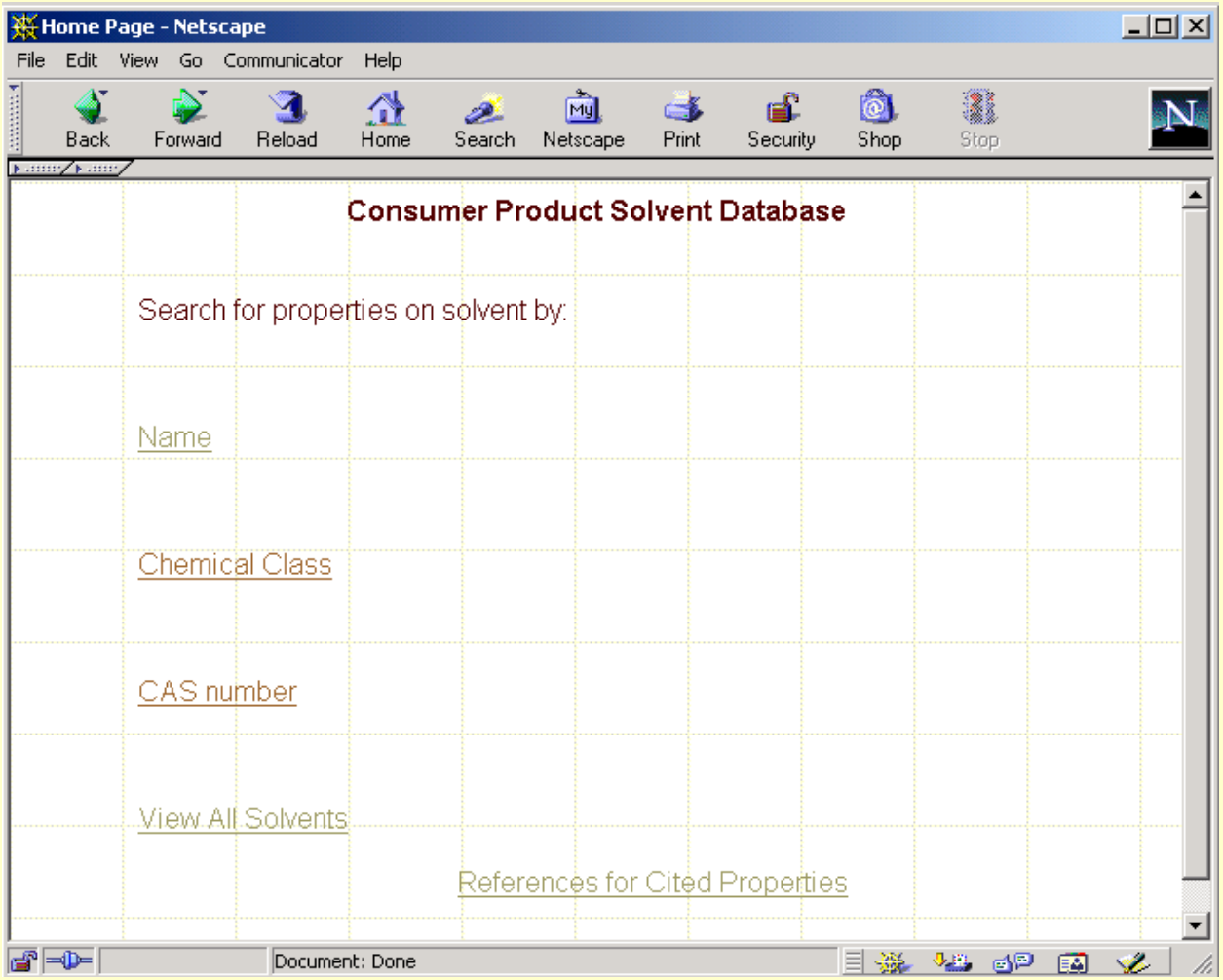
Database Home Page



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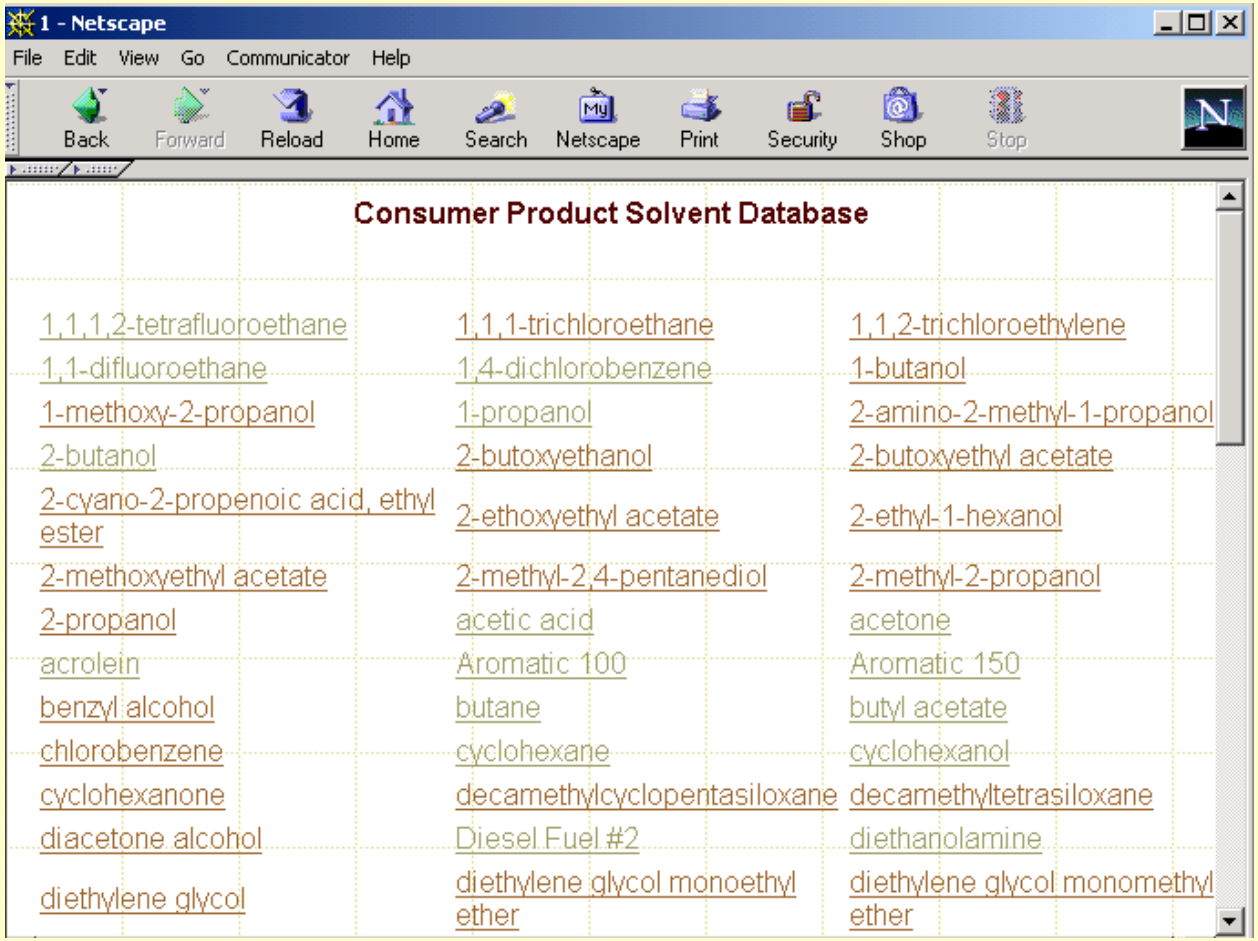
Database Master List



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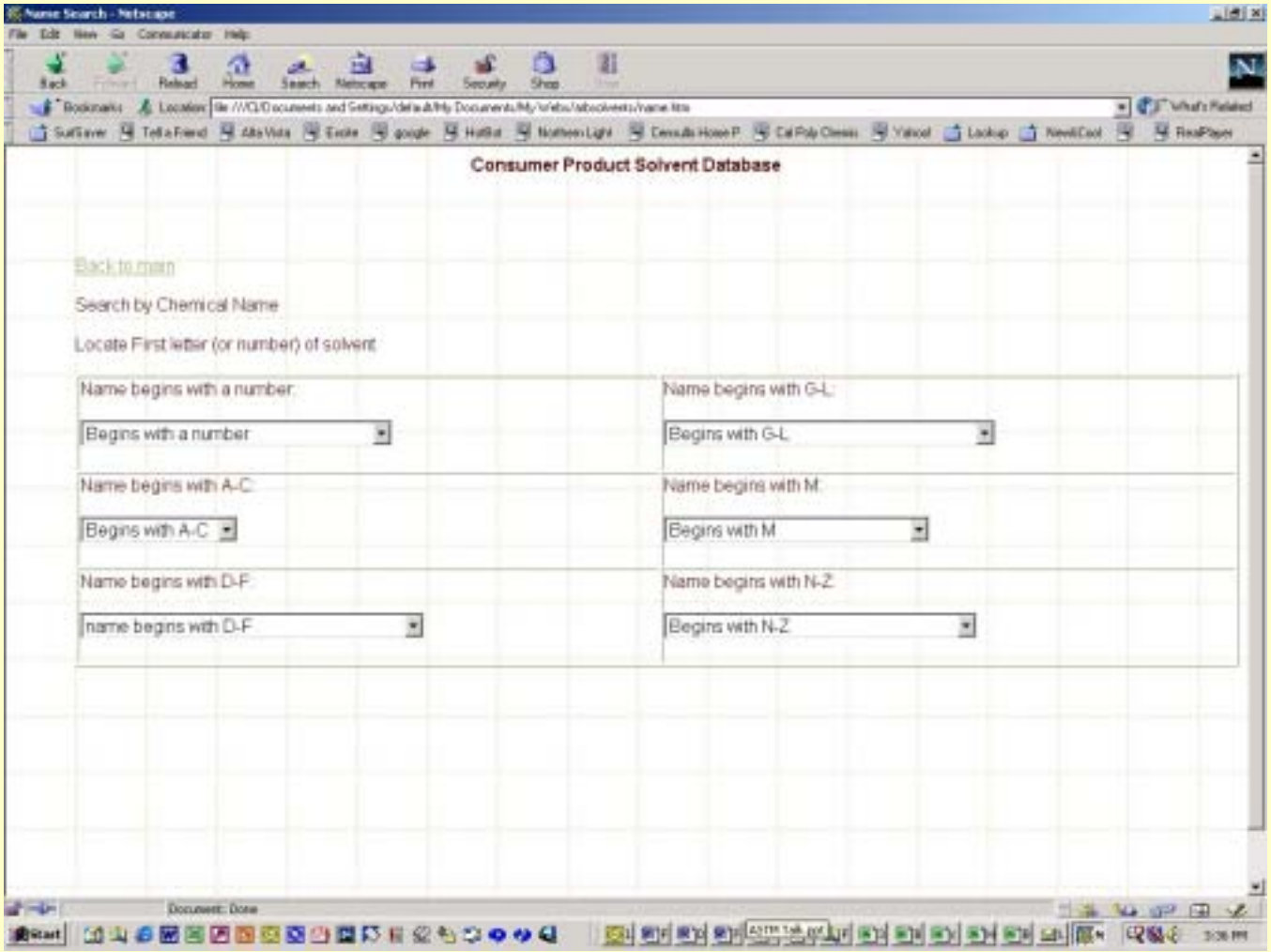
Database Search by Name Form



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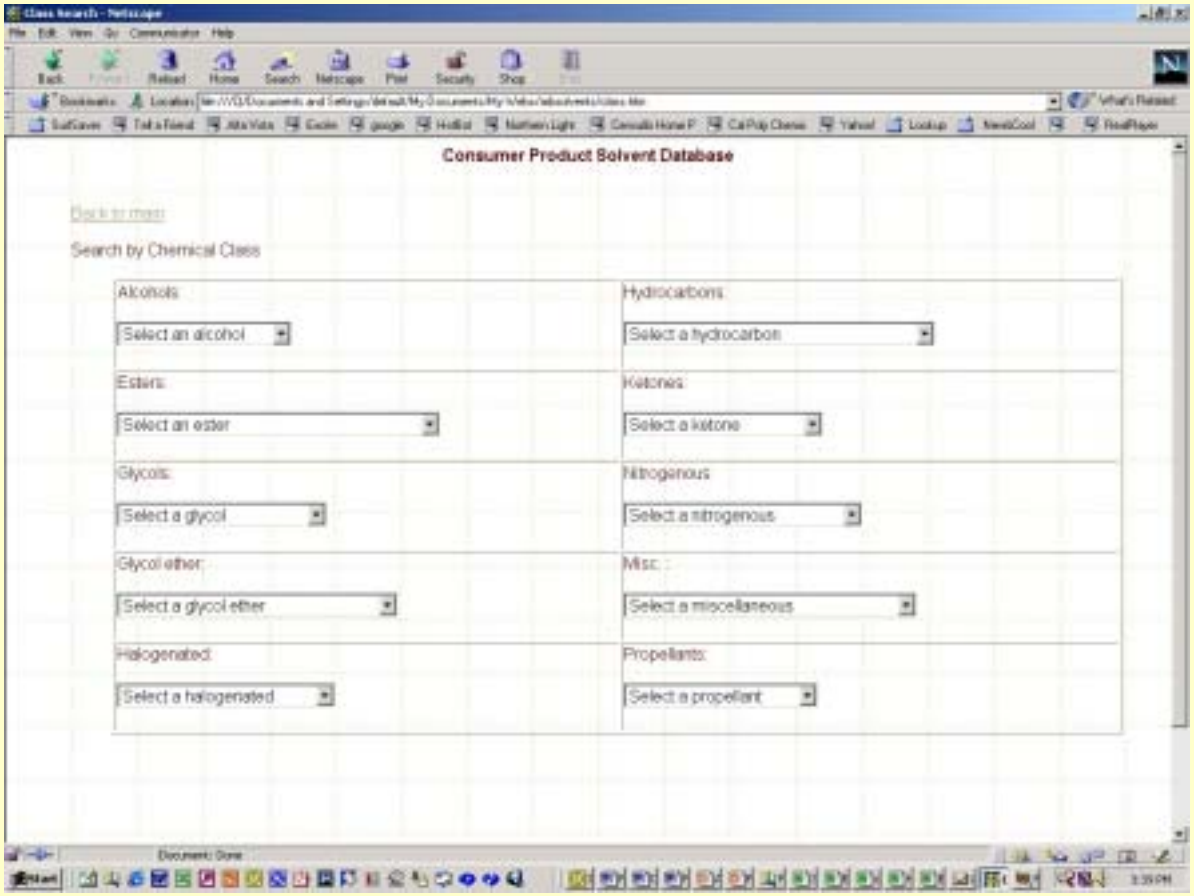

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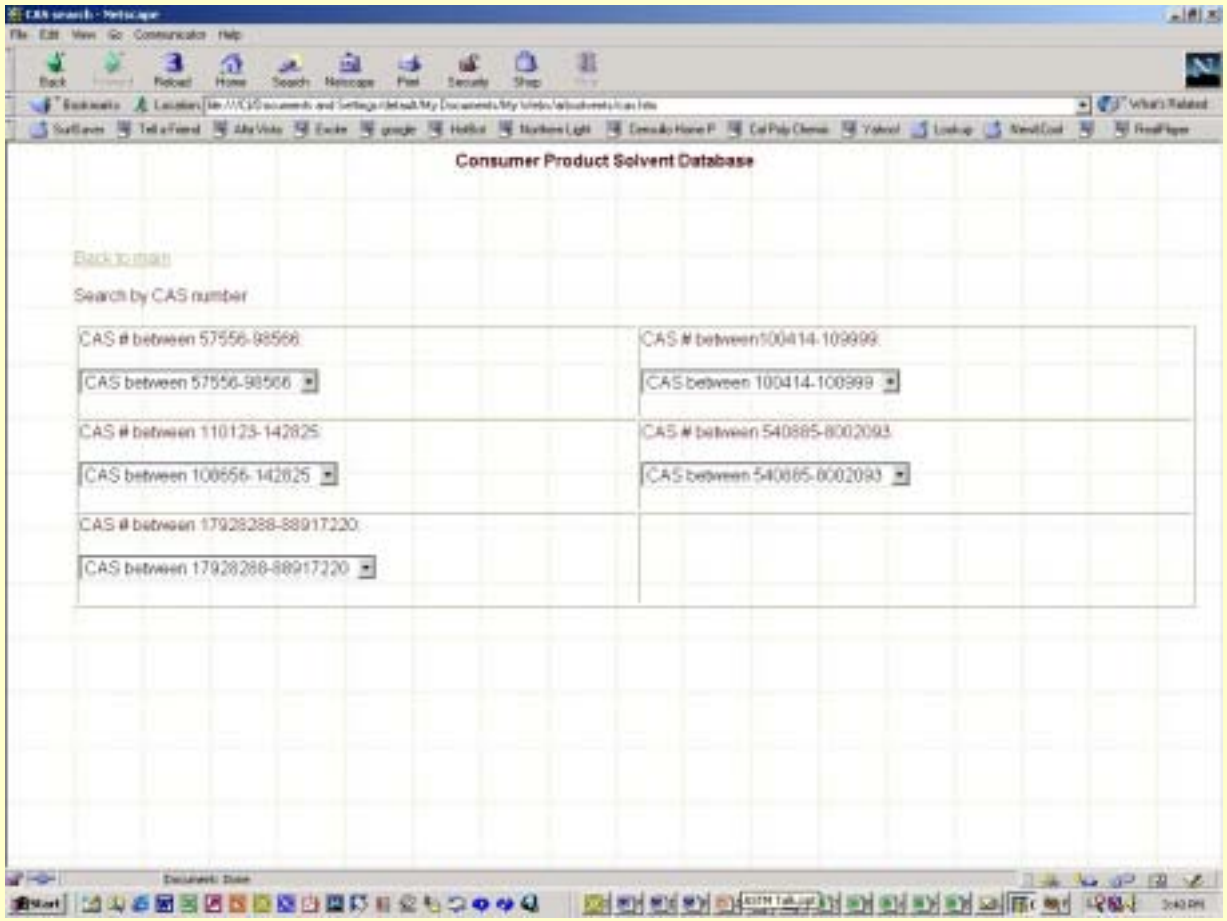
Database Search by CAS Number Form



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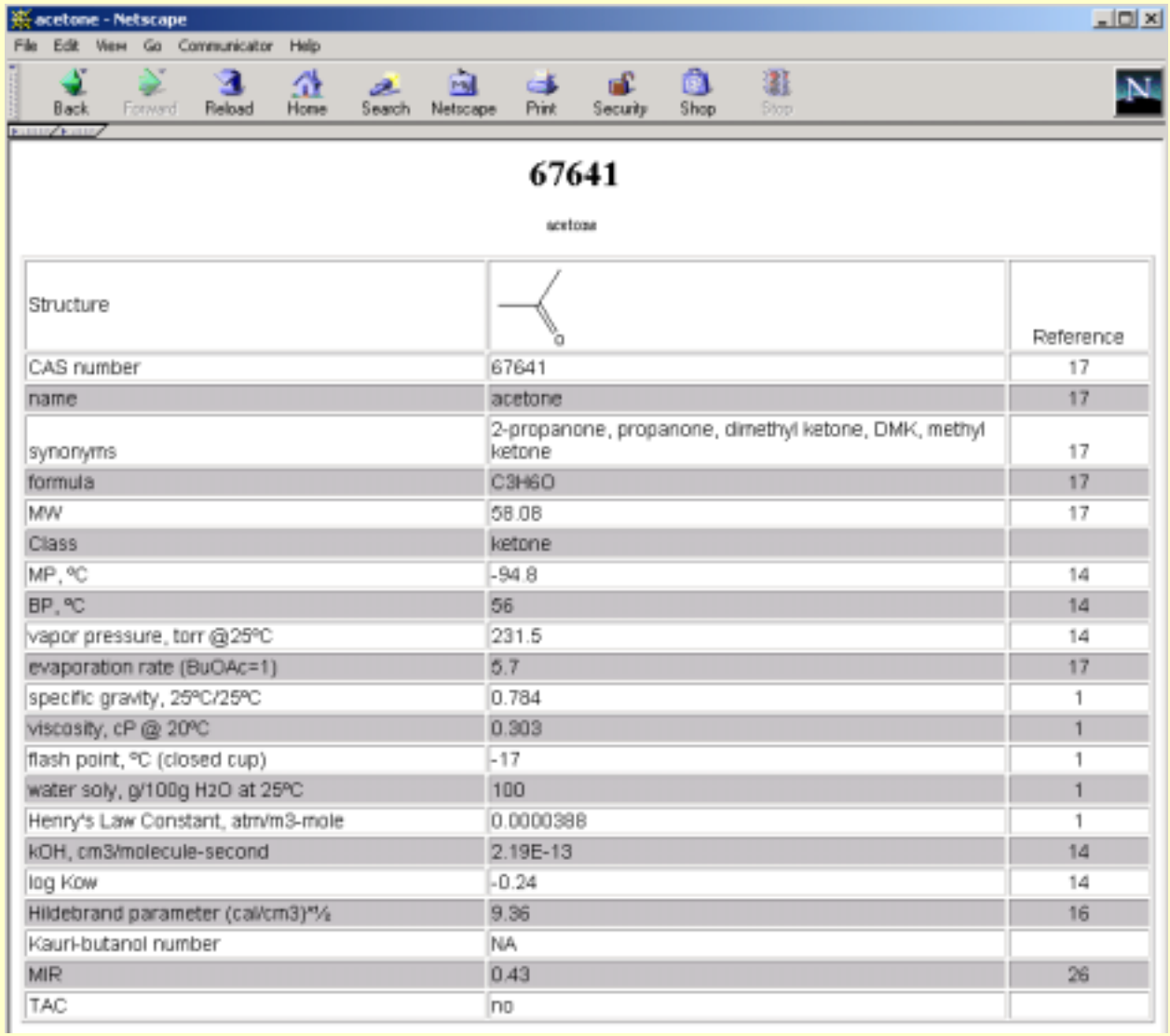
Database Sample Record



67641

acetone

Structure		Reference
CAS number	67641	17
name	acetone	17
synonyms	2-propanone, propanone, dimethyl ketone, DMK, methyl ketone	17
formula	C3H6O	17
MW	58.08	17
Class	ketone	
MP, °C	-94.8	14
BP, °C	56	14
vapor pressure, torr @25°C	231.5	14
evaporation rate (BuOAc=1)	5.7	17
specific gravity, 25°C/25°C	0.784	1
viscosity, cP @ 20°C	0.303	1
flash point, °C (closed cup)	-17	1
water soly, g/100g H2O at 25°C	100	1
Henry's Law Constant, atm/m3-mole	0.0000388	1
kOH, cm3/molecule-second	2.19E-13	14
log Kow	-0.24	14
Hildebrand parameter (cal/cm3)**½	9.36	16
Kauri-butanol number	NA	
MIR	0.43	26
TAC	no	

ASTM Designations for Hydrocarbon Solvents

- VM&P Naphthas
  - Type I (regular)
  - Type II (high flash)
  - Type III (odorless)
  - Type IV (low aromatic)
- Mineral Spirits and Stoddard Solvent
  - Type IA,B,C (full range)
  - Type IIA,B,C (high flash point)
  - Type IIIC (odorless)
  - Type IVA,B,C (low dry point)
- High Flash Aromatic Naphtha
  - Type I
  - Type II

“Investigation of Low-Reactivity Solvents”

ASTM Designations for Hydrocarbon Solvents

VM&P Naphthas, according to ASTM Specification D 3735-96				
	Type I	Type II	Type III	Type IV
Commercial reference	Regular	High Flash	Odorless	Low Aromatic
Appearance	Clear and free of suspended matter and undissolved water			
Bromine number, max	5	5	5	5
Color	Not darker than +28 (Saybolt scale), or 10 (platinum-cobalt scale)			
Aromatics, volume %, max	20	20	1	2
Copper corrosion, max rating	1	1	1	1
Distillation, 0/C:				
Initial boiling point, min	113	138	113	113
50% recovered, max	129	160	129	129
Dry point, max	154	177	154	154
Flash point, min	4	27	4	4
Kauri-butanol value:				
min	32			
max	45	45	38	38
Odor	nonresidual	nonresidual	nonresidual	nonresidual
Apparent specific gravity, 25/25C:				
min	0.709	0.726	0.709	0.709
max	0.786	0.786	0.754	0.754

“Investigation of Low-Reactivity Solvents”

ASTM Designations for Hydrocarbon Solvents

Mineral Spirits & Stoddard Solvent, according to ASTM Specification D 235-95								
Note: Mineral Spirits are called "Stoddard Solvents" when used for dry cleaning								
	Type I Full Range Mineral Spirits			Type II High Flash Point			Type III Odorless	
	Class A	Class B	Class C	Class A	Class B	Class C		Class C
Aromatic Content, range, vol%	8-22	2-8 max	0-2	8-22	2-8 max	0-2		0-0.25
Commercial reference	regular	rule 66	low aromatic	regular	rule 66	low aromatic		odorless
Appearance	All - clear and free of suspended matter							
Flash Point, 0/C, min	38	38	38	61	61	61		38
Color, min	All - not darker than +25 (Saybolt Scale) or 25 (Pt-Co Scale)							
Kauri-butanol value:								
min	29	29	28	29	29	28		.....
max	45	45	40	45	45	40		29
Bromine number, max	5	1	0.1	5	1	0.1		0.1
Odor	All - characteristic, as agreed between purchaser and supplier							
Doctor test	All - negative							
Distillation, 0/C								
Initial boiling point, min	149	149	149	177	177	177		149
50% Recovered, max	182	182	182	199	199	199		196
Dry point, max	213	213	213	213	213	213		213
Residue from distillation:								
Vol %, max	All - 1.5							
Acidity	All - neutral							
Copper corrosion, max rating	All - 2A							
Apparent Specific Gravity, 15.6/15.6C:								
min	0.754	0.754	0.754	0.768	0.768	0.768		0.740
max	0.820	0.810	0.800	0.820	0.810	0.800		0.775

“Investigation of Low-Reactivity Solvents”

ASTM Designations for Hydrocarbon Solvents

High Flash Aromatic Naphthas, Classified according to ASTM Specification D 3734-96							
	Type I	Type II					
Commercial reference	Aromatic 100	Aromatic 150					
Appearance	All - clear of suspended matter and undissolved water						
Color	All - no darker than +28 (Saybolt scale) or 10 (Pt-Co scale)						
Aromatics, volume %, min	90	90					
Copper corrosion, 0.5 h at 100C	All - no iridescence, discoloration, or gray or black deposit on copper strip						
Distillation, 0/C							
Initial bopiling point, min	149	177					
50 % recovered, max	168	196					
Dry point, max	179	216					
Flash point, 0/C, min	38	61					
Kauri-butanol value, min	87	85					
Mixed aniline point, max	60	65					
Odor	All - characteristic, as agreed between purchaser and supplier						
Apparent specific gravity, 25/25C	0.857	0.873					
	0.874	0.903					

“Investigation of Low-Reactivity Solvents”

ASTM Designations for Hydrocarbon Solvents

VM&P Naphthas, according to ASTM Specification D 3735-96				
	Type I	**Type II**	**Type III**	**Type IV**
Commercial reference	Regular	High Flash	Odorless	Low Aromatic
Appearance	Clear and free of suspended matter and undissolved water			
Bromine number, max	5	5	5	5
Color	Not darker than +28 (Saybolt scale), or 10 (platinum-cobalt scale)			
Aromatics, volume %, max	20	20	1	2
Copper corrosion, max rating	1	1	1	1
Distillation, 0/C:				
Initial boiling point, min	113	138	113	113
50% recovered, max	129	160	129	129
Dry point, max	154	177	154	154
Flash point, min	4	27	4	4
Kauri-butanol value:				
min	32			
max	45	45	38	38
Odor	nonresidual	nonresidual	nonresidual	nonresidual
Apparent specific gravity, 25/25C:				
min	0.709	0.726	0.709	0.709
max	0.786	0.786	0.754	0.754

“Investigation of Low-Reactivity Solvents”

ASTM Designations for Hydrocarbon Solvents

Mineral Spirits & Stoddard Solvent, according to ASTM Specification D 235-95				
Note: Mineral Spirits are called "Stoddard Solvents" when used for dry cleaning				
	Type I Full Range Mineral Spirits			
	Class A	**Class B**	**Class C**	
Aromatic Content, range, vol%	8-22	2-8 max	0-2	
Commercial reference	regular	rule 66	low aromatic	
Appearance	All - clear and free of suspended matter			
Flash Point, 0/C, min	38	38	38	
Color, min	All - not darker than +25 (Saybolt Scale) or 25 (Pt-Co Scale)			
Kauri-butanol value:				
min	29	29	28	
max	45	45	40	
Bromine number, max	5	1	0.1	
Odor	All - characteristic, as agreed between purchaser and supplier			
Doctor test	All - negative			
Distillation, 0/C				
Initial boiling point, min	149	149	149	
50% Recovered, max	182	182	182	
Dry point, max	213	213	213	
Residue from distillation:				
Vol %, max	All - 1.5			
Acidity	All - neutral			
Copper corrosion, max rating	All - 2A			
Apparent Specific Gravity, 15.6/15.6C:				
min	0.754	0.754	0.754	
max	0.820	0.810	0.800	

“Investigation of Low-Reactivity Solvents”

ASTM Designations for Hydrocarbon Solvents

Mineral Spirits	**Type II High Flash Point**			**Type III Odorless**
	Class A	**Class B**	**Class C**	**Class C**
Aromatic Content, range, vol%	8-22	2-8 max	0-2	0-0.25
Commercial reference	regular	rule 66	low aromatic	odorless
Appearance				
Flash Point, 0/C, min	61	61	61	38
Color, min				
Kauri-butanol value:				
min	29	29	28	…..
max	45	45	40	29
Bromine number, max	5	1	0.1	0.1
Odor				
Doctor test				
Distillation, 0/C				
Initial boiling point, min	177	177	177	149
50% Recovered, max	199	199	199	196
Dry point, max	213	213	213	213
Residue from distillation:				
Vol %, max				
Acidity				
Copper corrosion, max rating				
Apparent Specific Gravity, 15.6/15.6C:				
min	0.768	0.768	0.768	0.740
max	0.820	0.810	0.800	0.775

“Investigation of Low-Reactivity Solvents”

ASTM Designations for Hydrocarbon Solvents

Mineral Spirits	**Type IV Low Dry Point**		
	Class A	**Class B**	**Class C**
Aromatic Content, range, vol%	8-22	2-8 max	0-2
Commercial reference	regular	rule 66	low aromatic
Appearance			
Flash Point, 0/C, min	38	38	38
Color, min			
Kauri-butanol value:			
min	29	29	28
max	45	45	40
Bromine number, max	5	1	0.1
Odor			
Doctor test			
Distillation, 0/C			
Initial boiling point, min	149	149	149
50% Recovered, max	174	174	174
Dry point, max	185	185	185
Residue from distillation:			
Vol %, max			
Acidity			
Copper corrosion, max rating			
Apparent Specific Gravity, 15.6/15.6C:			
min	0.754	0.754	0.754
max	0.810	0.800	0.790

“Investigation of Low-Reactivity Solvents”

ASTM Designations for Hydrocarbon Solvents

High Flash Aromatic Naphthas, according to ASTM Specification D 3734-96

	Type I	Type II		
Commercial reference	Aromatic 100	Aromatic 150		
Appearance	All - clear of suspended matter and undissolved water			
Color	All - no darker than +28 (Saybolt scale) or 10 (Pt-Co scale)			
Aromatics, volume %, min	90	90		
Copper corrosion, 0.5 h at 100C	All - no iridescence, discoloration, or gray or black deposit on copp			
Distillation, 0/C				
Initial bopiling point, min	149	177		
50 % recovered, max	168	196		
Dry point, max	179	216		
Flash point, 0/C, min	38	61		
Kauri-butanol value, min	87	85		
Mixed aniline point, max	60	65		
Odor	All - characteristic, as agreed between purchaser and supplier			
Apparent specific gravity, 25/25C	0.857	0.873		
	0.874	0.903		

“Investigation of Low-Reactivity Solvents”

Task: Chemical Speciation of Hydrocarbon Solvents

Sample Selection

- Hydrocarbon mixtures targeted
- 42 samples selected and analyzed

"Investigation of Low-Reactivity Solvents"

Task: Chemical Speciation of Hydrocarbon Solvents

Sample Types

product name	CalPolyID	product name	CalPolyI
VM&P naphtha	CP1	VM&P Naphtha	CP23
300-66 solvent, Mineral Spirits 66	CP2	VM&P Naphtha	CP24
Light HC solvent	CP3	Mineral Spirits	CP25
VM&P naphtha HT	CP4	Mineral Spirits	CP26
Lactol Spirits	CP5	xylene	CP27
Mineral Spirits	CP6	light naphtha solvent	CP28
Aromatic 100	CP7	aliphatic petroleum distillates	CP29
Aromatic 150	CP8	VM&P naphtha	CP30
Mineral Spirits	CP10	Aromatic 100	CP31
Mineral Spirits	CP11	Aromatic 150	CP32
Mineral Spirits	CP12	Mineral Spirits	CP33
Aromatic 100	CP13	xylene	CP34
VM&P Naphtha	CP14	VM&P naphtha	CP35
aliphatic petroleum distillates	CP15	Aromatic 100	CP36
aliphatic petroleum distillates	CP16	Aromatic 150	CP37
Aromatic 150	CP17	isoparaffinic hydrocarbon	CP38
aliphatic petroleum distillates	CP18	paraffinic petroleum distillate	CP39
xylene	CP19	Xylene	CP40
Stoddard Solvent	CP20	Xylene	CP41
Aromatic 100	CP21	Aromatic 100	CP42
Aromatic 150	CP22	Mineral spirits	CP43

“Investigation of Low-Reactivity Solvents”

Task: Chemical Speciation of Hydrocarbon Solvents

Analytical Methodologies

- All samples run on 100 m capillary PDMS column, using GC-FID
- All samples run on 100 m capillary PDMS column, using GC-MS
- All samples run on 60 m capillary Carbowax, using GC-FID
- Many samples used SPME for verification of aromatic peaks

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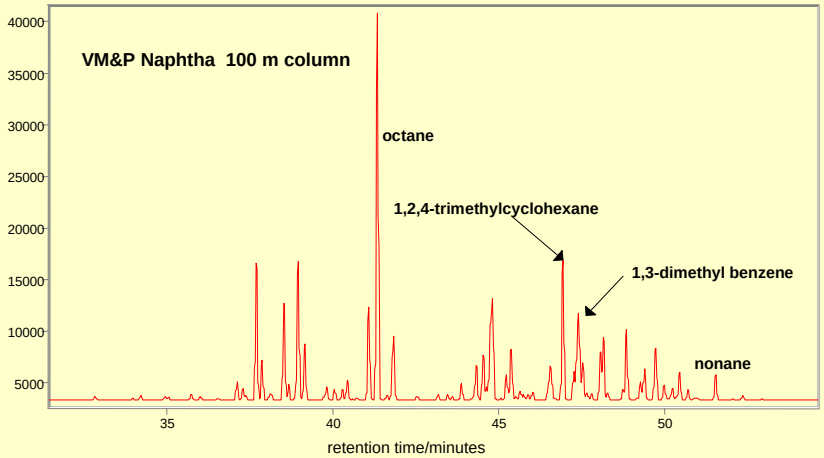
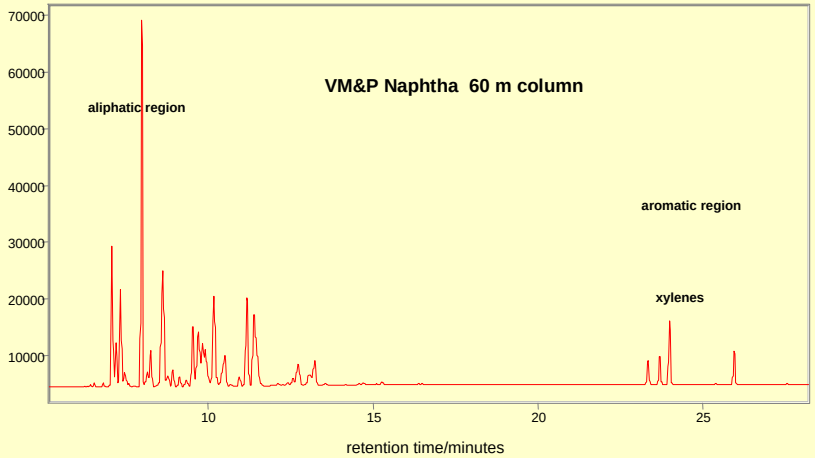
Task: Chemical Speciation of Hydrocarbon Solvents

Comparison of PDMS and Carbowax Columns





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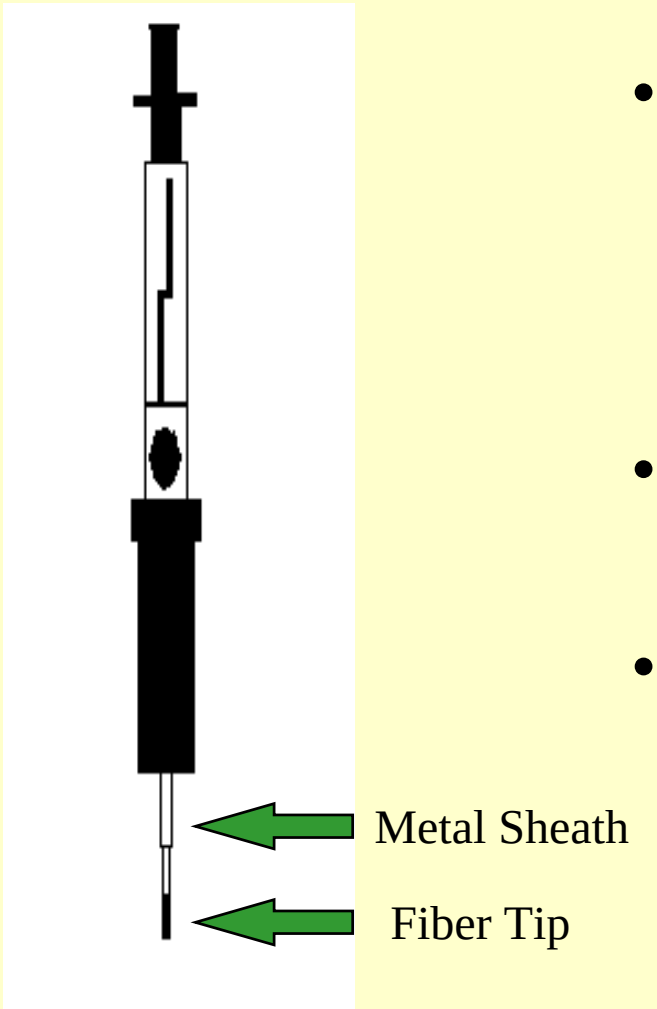
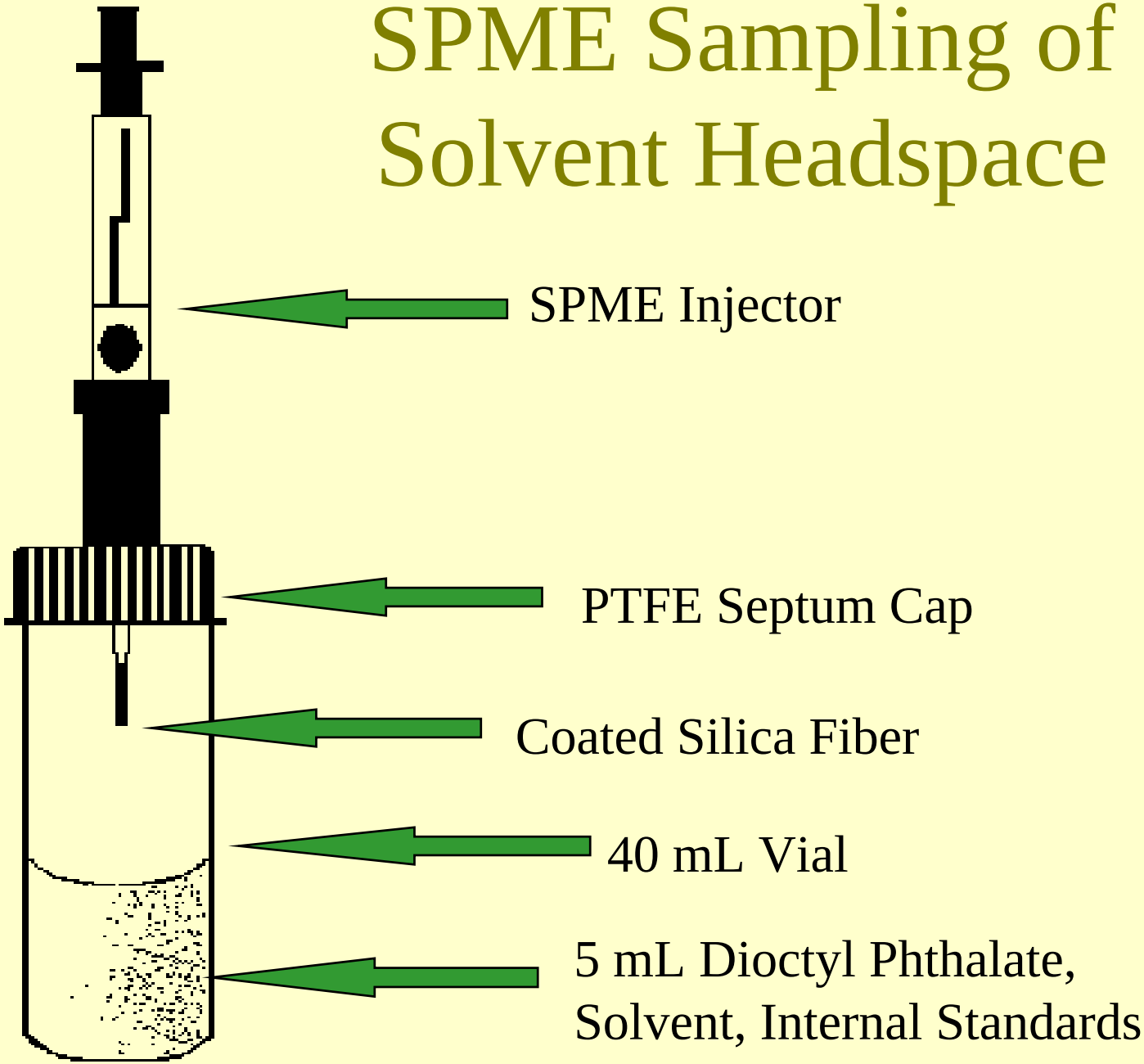
Task: Chemical Speciation of Hydrocarbon Solvents

Sampling With SPME



- Silica fiber tip coated with Carbowax-divinylbenzene (or other adsorbing material) is placed in contact with solvent headspace
- Solvent molecules in headspace are adsorbed and concentrated on fiber
- Fiber is withdrawn into protective metal sheath and inserted into hot GC injection port where solvent molecules are thermally desorbed onto column

SPME Sampling of Solvent Headspace



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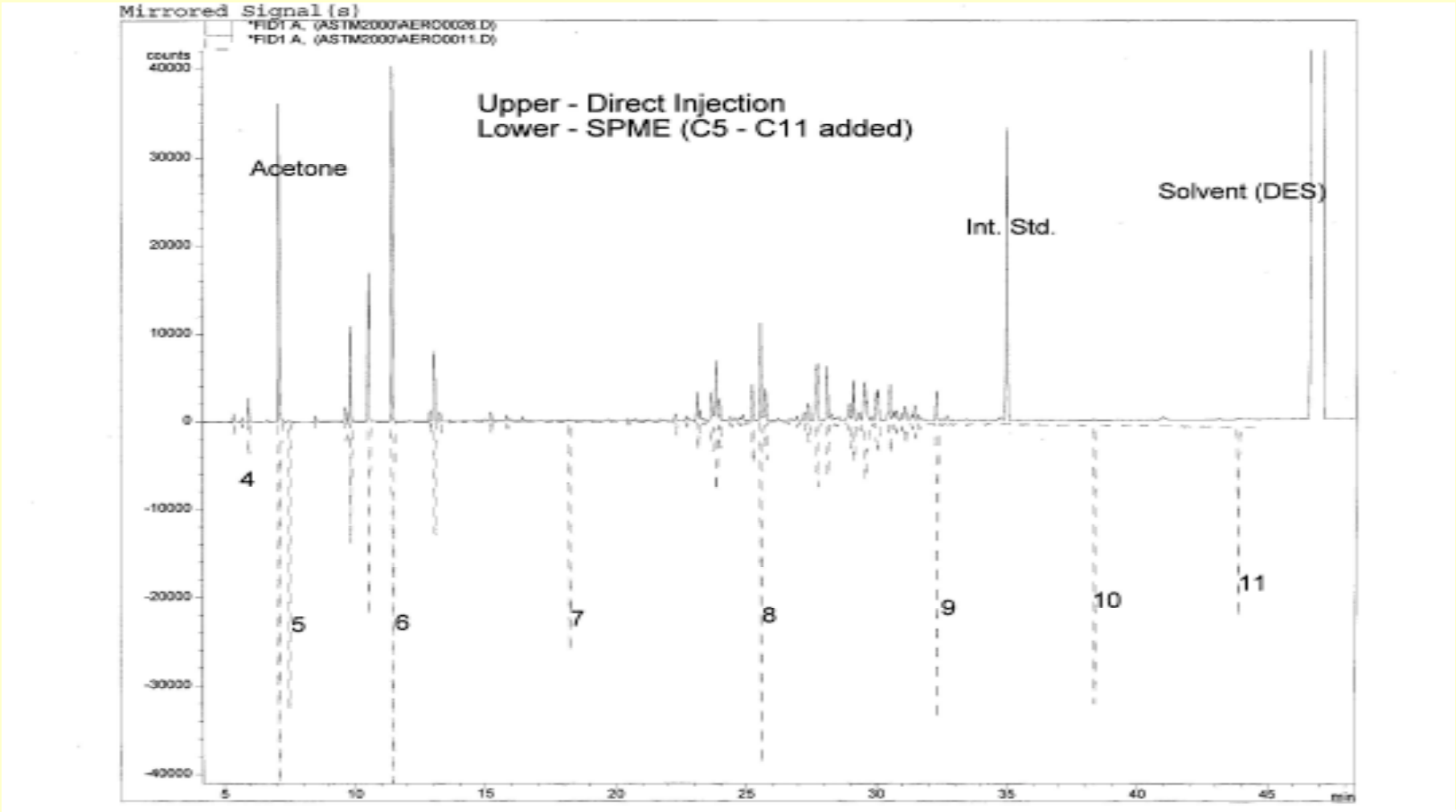
SPME vs. Direct Injection for Hydrocarbons

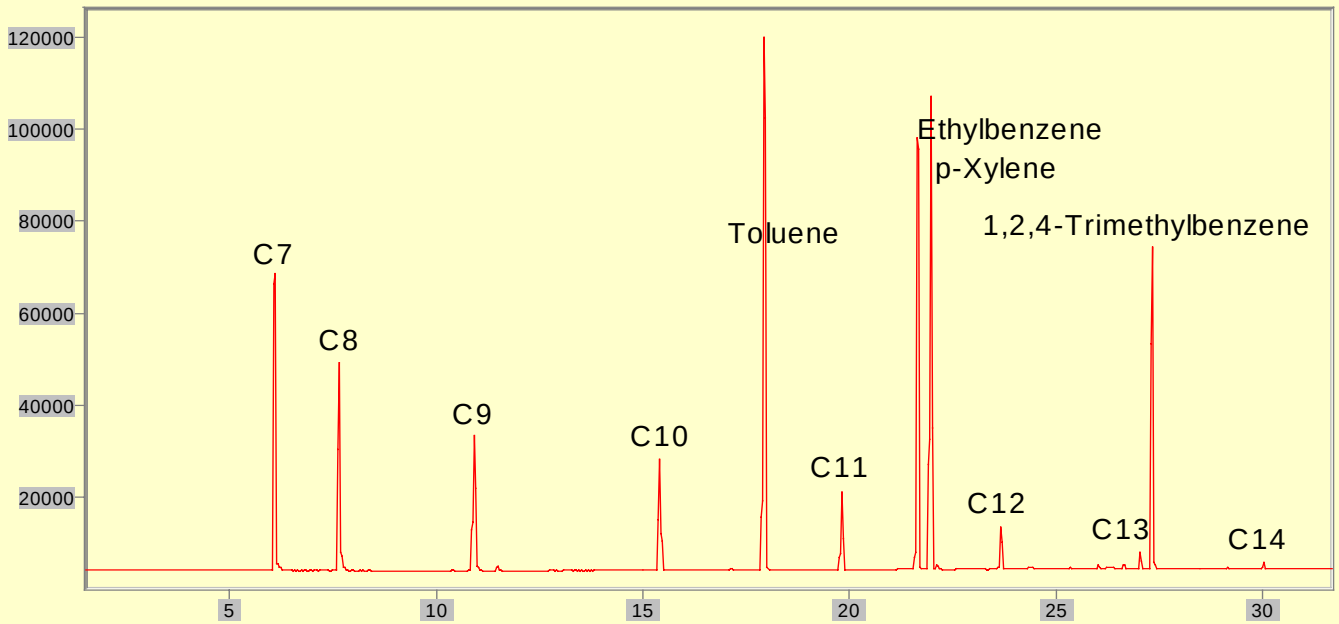


“Investigation of Low-Reactivity Solvents”

Task: Chemical Speciation of Hydrocarbon Solvents

Selectivity of SPME for Aromatics, Carbowax Column

Equal masses of each component, 25^0C



Counts / Minutes
File # 2 = FID1A
7-14/aromat/SPME \max

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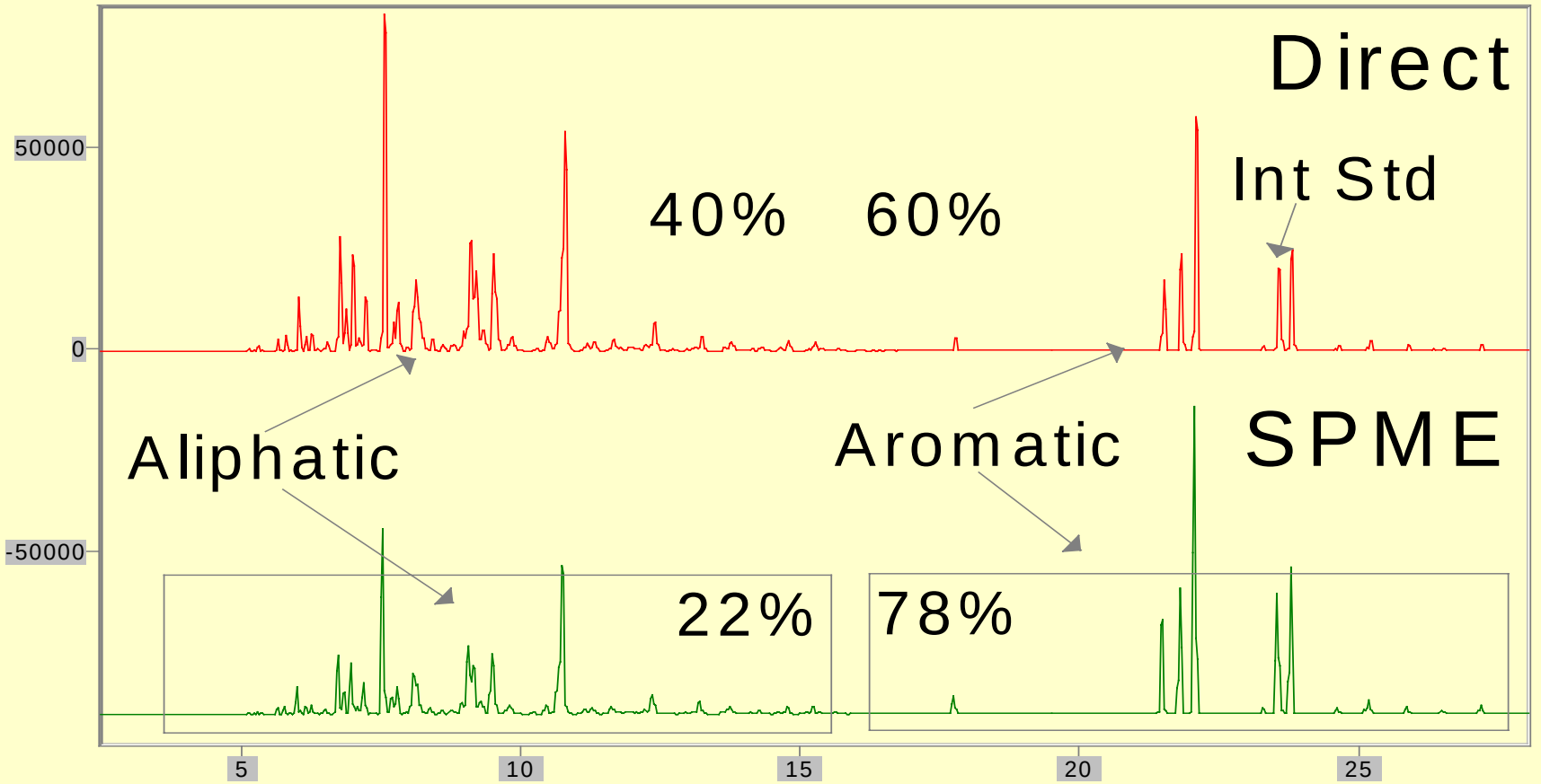
10/28/00 1:16 PM Res=None

“Investigation of Low-Reactivity Solvents”

Task: Chemical Speciation of Hydrocarbon Solvents

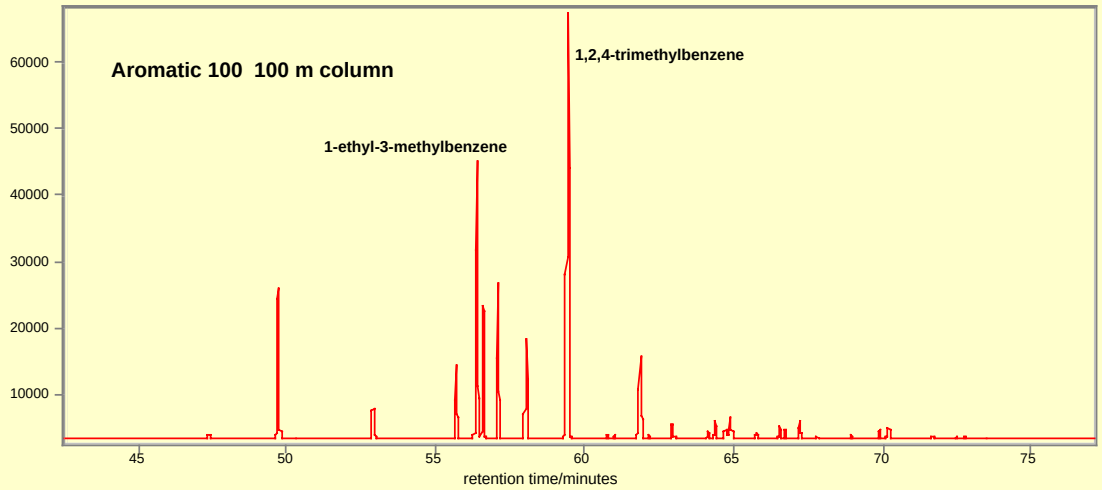
SPME vs. Direct Injection for Hydrocarbons

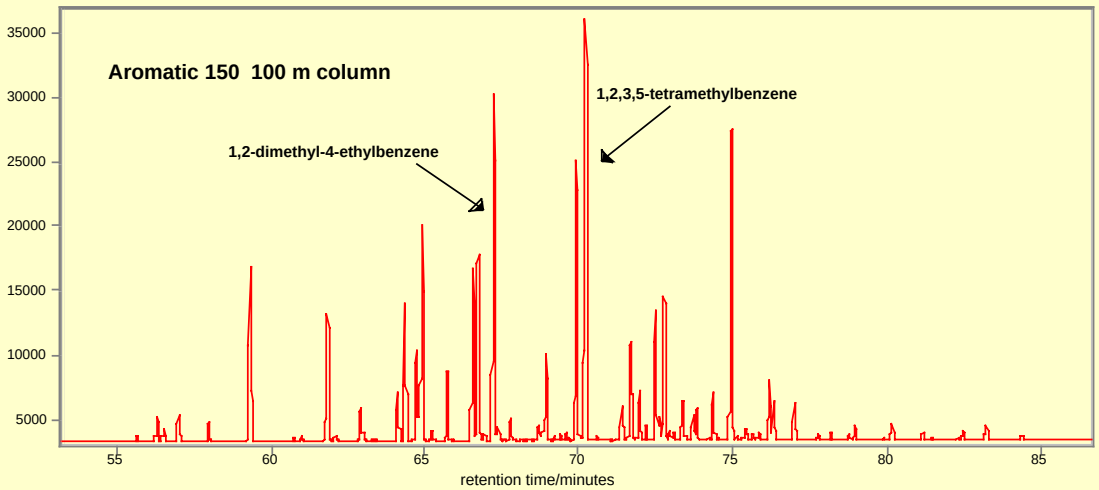
VM&P Naphtha and xylenes on Carbowax Column



“Investigation of Low-Reactivity Solvents”

Representative Chromatograms





“Investigation of Low-Reactivity Solvents”

Task: Chemical Speciation of Hydrocarbon Solvents

Format for Results

- Summary sheets by carbon number
  - Normal paraffins
  - Isoparaffins
  - Cyclic paraffins
  - Unidentified paraffins
  - Aromatics
- Detailed species profiles

“Investigation of Low-Reactivity Solvents”

Task: Chemical Speciation of Hydrocarbon Solvents

Summary sheets by carbon number

Product	Distillation Range	Carbon Number Distribution, Wt%															Composition,Wt%
		C 5	C 6	C 7	C 8	C 9	C 10	C 11	C 12	C 13	C 14	C 15	C 16	C 17	C 18	C19	Total	
																		n-PAR
																		i-PAR
																		c-PAR
																		u-PAR
																		AROM

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Species Profile Format

CP5, Lactol Spirits	CAS#	fraction
Hexane, 2,2-dimethyl	590738	0.1687
Cyclopentane, 1,2-	822504	0.0987
Cyclopentane, 1,2,3-	19374460	0.0799
Heptane	142825	0.0723
Toluene	108883	0.0654
Cyclopentane, 1,3-	1759586	0.0617
Cyclopentane, 1,3-	2532583	0.0566
Cyclopentane, 1,2,4-	18679306	0.0529
c-Paraffin, C7		0.0421
Cyclopentane, ethyl	1640897	0.0386
Cyclopentane, methyl	96377	0.0379
Hexane, 3-methyl	589344	0.0348
Cyclopentane, 1,1,3-	4516692	0.0342
Cyclohexane, methyl	108872	0.0242
Hexane, 2-methyl	591764	0.0217
Pentane, 2,3-dimethyl	565593	0.0182
Cyclopentane, 1,1-	1638262	0.0147
Hexane, 2,3-dimethyl	584941	0.0095
Hexane	110543	0.009
Hexane, 2,4-dimethyl	116502444	0.0088
Heptane, 2-methyl	592278	0.0062
Cyclohexane, 1,4-	2207047	0.0049
Hexane, 3-ethyl	619998	0.0044
Pentane, 2,4-dimethyl	108087	0.0035
Pentane, 2,3,4-trimethyl	565753	0.0032
Benzene	71432	0.0031
Hexane, 2,3-dimethyl	584941	0.003
Cyclohexane, 1,1-	590669	0.0024
Hexane, 3,4-dimethyl	583482	0.002
Hexane, 3,3-dimethyl	563166	0.002
Cyclopentane, 1-ethyl-2-	930892	0.0016
Cyclopentane, 1,1,2-	4259001	0.0015
Pentane, 2,2-dimethyl	590352	0.0014
Pentane, 3,3-dimethyl	562492	0.0013
Pentane, 3-methyl	96140	0.0013
Cyclopentane, 1-ethyl-1-	16747505	0.001
i-Paraffin, C7		0.001
Pentane, 2-methyl	107835	0.001
Heptane, 3-methyl	589811	0.0009
Cyclopentane, 1-ethyl-1-	16747505	0.0009
Octane	111659	0.0008
Cyclohexane, 1,3-	638040	0.0007
c-Paraffin, C8		0.0006
Butane, 2,2,3-trimethyl	464062	0.0005
Cyclohexane, 1,4-	624293	0.0004
u-Paraffin, C8		0.0003
Cyclohexane, 1,2-	6876239	0.0001
Total		**1.0000**

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Final Report Presented by

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