



This presentation shows a variety of application which can be performed using Supelco ionic liquid GC columns.

Agenda

- Chromatograms
- Summary / Related Products / Resources

- Environmental
 - Petroleum
 - Biofuel
 - Chemical
 - Agriculture
 - Food and Beverage
 - Flavor and Fragrance
 - Clinical
 - General Analytical

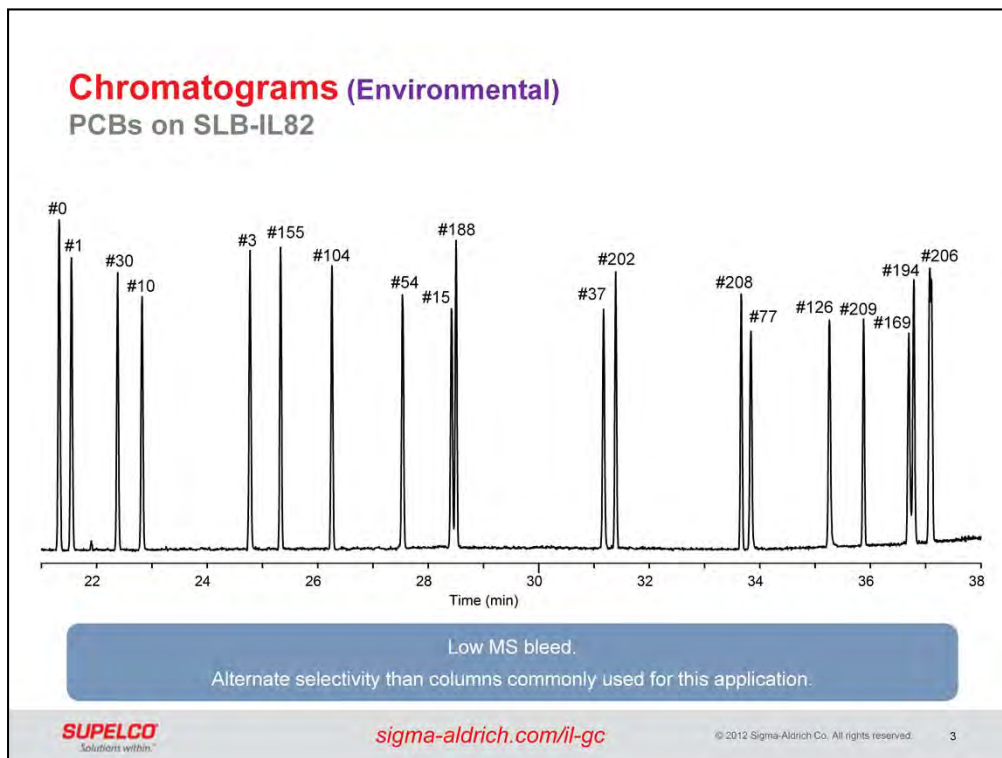
Analyte IDs and GC conditions are included in the speaker notes for most chromatograms. Otherwise, enter chromatogram ID from speaker notes into the search bar at <sigma-aldrich.com>.

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Chromatograms – Environmental Applications



Polychlorinated biphenyls (PCBs) were widely used as insulating fluids for transformers and capacitors from the 1930's into the 1980's. Their use was stopped when it was discovered they are environmental contaminants. Because PCBs do not decompose readily, they are classified as persistent organic pollutants (POPs), and can be found in soil, oil, water, and air. This chromatogram of 19 PCBs was analyzed on the SLB-IL82. In addition to the low level of MS bleed, the SLB-IL82 offers alternate selectivity than the columns commonly used for this application.

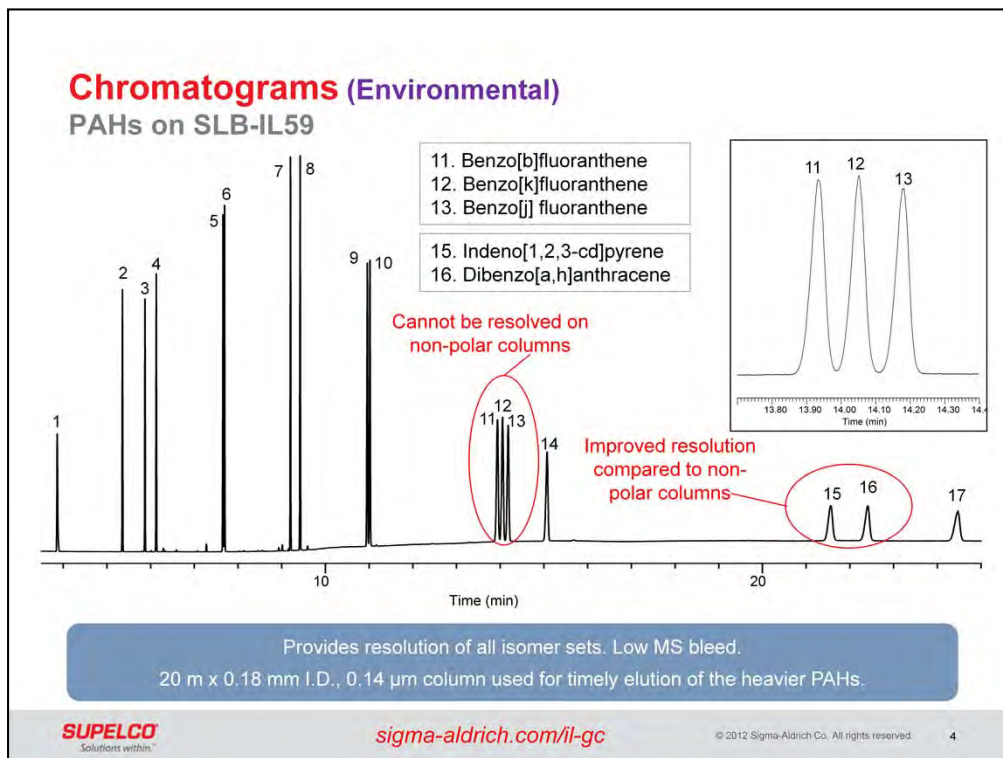
Peak IDs

- #0 = Biphenyl
- #1 = 2-monochlorobiphenyl
- #3 = 4-monochlorobiphenyl
- #10 = 2,6-dichlorobiphenyl
- #15 = 4,4'-dichlorobiphenyl
- #30 = 2,4,6-trichlorobiphenyl
- #37 = 3,4,4'-trichlorobiphenyl
- #54 = 2,2',6,6'-tetrachlorobiphenyl
- #77 = 3,3',4,4'-tetrachlorobiphenyl
- #104 = 2,2',4,6,6'-pentachlorobiphenyl
- #126 = 3,3',4,4',5-pentachlorobiphenyl
- #155 = 2,2',4,4',6,6'-hexachlorobiphenyl
- #169 = 3,3',4,4',5,5'-hexachlorobiphenyl
- #188 = 2,2',3,4',5,6,6'-heptachlorobiphenyl
- #194 = 2,2',3,3',4,4',5,5'-octachlorobiphenyl
- #202 = 2,2',3,3',5,5',6,6'-octachlorobiphenyl
- #206 = 2,2',3,3',4,4',5,5',6-nonachlorobiphenyl
- #208 = 2,2',3,3',4,5,5',6,6'-nonachlorobiphenyl
- #209 = Decachlorobiphenyl

Conditions

- column: SLB-IL82, 30 m x 0.25 mm I.D., 0.20 μ m (29479-U)
- oven: 50 $^{\circ}$ C (2 min), 5 $^{\circ}$ C/min to 260 $^{\circ}$ C
- inj. temp.: 250 $^{\circ}$ C
- detector: MSD, m/z = 100-550
- carrier gas: helium, 1.0 mL/min
- injection: 1 μ L, splitless (splitter open at 1 min)
- liner: 4 mm I.D., split/splitless type, single taper design
- sample: PCB congener mix, each analyte at 2.5 ppm in n-hexane

[Chromatogram ID = G006237]



Polycyclic aromatic hydrocarbons (PAHs) are produced as by-products of burning fuel. Several PAHs are identified as carcinogens. The PAHs of interest include several isomer sets. This chromatogram of 19 PAHs on the SLB-IL59 highlights the ability of this column to provide resolution of all isomer sets, and exhibit low MS bleed. A 20 m x 0.18 mm I.D., 0.14 µm column was used for the timely elution of the heavier PAHs.

Peak IDs

1. Naphthalene
2. Acenaphthene
3. Acenaphthylene
4. Fluorene
5. Phenanthrene
6. Anthracene
7. Fluoranthene
8. Pyrene
9. Benzo[a]anthracene
10. Chrysene
11. Benzo[b]fluoranthene
12. Benzo[k]fluoranthene
13. Benzo[j] fluoranthene
14. Benzo[a]pyrene
15. Indeno[1,2,3-cd]pyrene
16. Dibenzo[a,h]anthracene
17. Benzo[g,h,i]perylene

Conditions

- column: SLB-IL59, 20 m x 0.18 mm I.D., 0.14 µm (custom)
- oven: 65 °C (0.5 min), 25 °C/min to 300 °C (20 min)
- inj. temp.: 265 °C
- carrier gas: helium, 50 psi constant pressure
- detector: MSD, interface at 300 °C, m/z = 50-500
- injection: 1 µL, splitless (1 min)
- liner: 4 mm I.D., split/splitless type, wool packed single taper FocusLiner design
- sample: each PAH at 10 µg/mL in methylene chloride

[Chromatogram ID = G006238]

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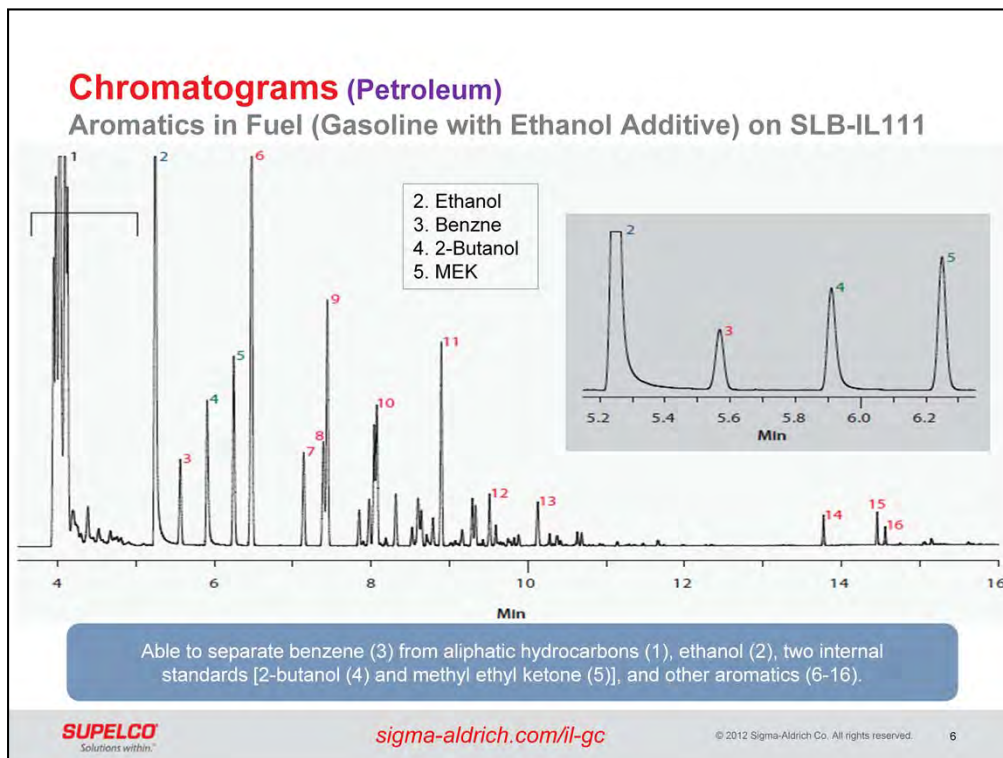
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Chromatograms – Petroleum Applications



Benzene is a carcinogen, and its level in gasoline should be monitored to reduce exposure to consumers and workers. Reformulated gasoline also contains oxygenates, additives designed to increase combustion and minimize emissions. To determine the level of benzene in reformulated gasoline, it must be resolved from aliphatics, other aromatics, oxygenates, and any internal standards. The SLB-IL111 can be used in a single column configuration to perform this application. This chromatogram is of reformulated gasoline with ethanol as the oxygenate, and two internal standards. A 60 m column was able to provide the resolution of benzene from all other components. Also note that the heavy constituents (methylnaphthalenes, peaks 15 and 16) elute in a timely manner with great peak shapes.

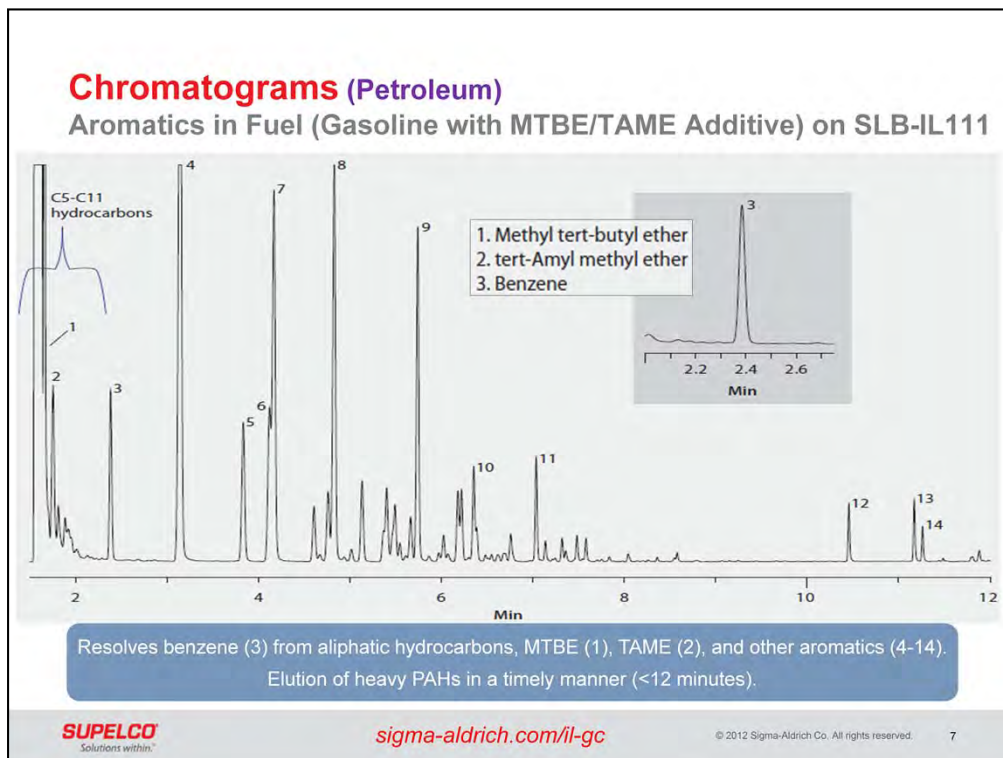
Peak IDs

1. C5-C11 Hydrocarbons
2. Ethanol
3. Benzene
4. 2-Butanol (int. std.)
5. Methyl ethyl ketone (int. std.)
6. Toluene
7. Ethylbenzene
8. p-Xylene
9. m-Xylene
10. o-Xylene
11. 1,2,4-Trimethylbenzene
12. 1,2,3-Trimethylbenzene
13. 1,2,4,5-Tetramethylbenzene
14. Naphthalene
15. 2-Methylnaphthalene
16. 1-Methylnaphthalene

Conditions

- column: SLB-IL111, 60 m x 0.25 mm I.D., 0.20 μ m (28928-U)
- oven: 50 °C (3 min), 15 °C/min to 265 °C (5 min)
- inj. temp.: 250 °C
- detector: FID, 275 °C
- carrier gas: helium, 30 cm/sec
- injection: 0.5 μ L, 200:1 split
- liner: 4 mm I.D., split type, wool packed single taper FocusLiner design
- sample: Premium unleaded gasoline, plus ethanol at 20% (v/v) and two internals each at 4% (v/v)

[Chromatogram ID = G005642]



This chromatogram is of reformulated gasoline with MTBE and TAME as oxygenates. A 30 m SLB-IL111 column was able to provide the resolution of benzene from all other components. Also note that the heavy constituents (methylnaphthalenes, peaks 13 and 14) elute in a timely manner with great peak shapes.

Peak IDs

1. Methyl tert-butyl ether (MTBE)
2. tert-Amyl methyl ether (TAME)
3. Benzene
4. Toluene
5. Ethylbenzene
6. p-Xylene
7. m-Xylene
8. o-Xylene
9. 1,2,4-Trimethylbenzene
10. 1,2,3-Trimethylbenzene
11. 1,2,4,5-Tetramethylbenzene
12. Naphthalene
13. 2-Methylnaphthalene
14. 1-Methylnaphthalene

Conditions

- column: SLB-IL111, 30 m x 0.25 mm I.D., 0.20 μ m (28927-U)
- oven: 50 $^{\circ}$ C (3 min), 15 $^{\circ}$ C/min to 265 $^{\circ}$ C (5 min)
- inj. temp.: 250 $^{\circ}$ C
- detector: FID, 275 $^{\circ}$ C
- carrier gas: helium, 30 cm/sec
- injection: 0.5 μ L, 200:1 split
- liner: 4 mm I.D., split/splitless type, wool packed single taper FocusLiner design
- sample: Premium unleaded gasoline, plus MTBE at 10% (v/v) and TAME at 1% (v/v)

[Chromatogram ID = G005866]

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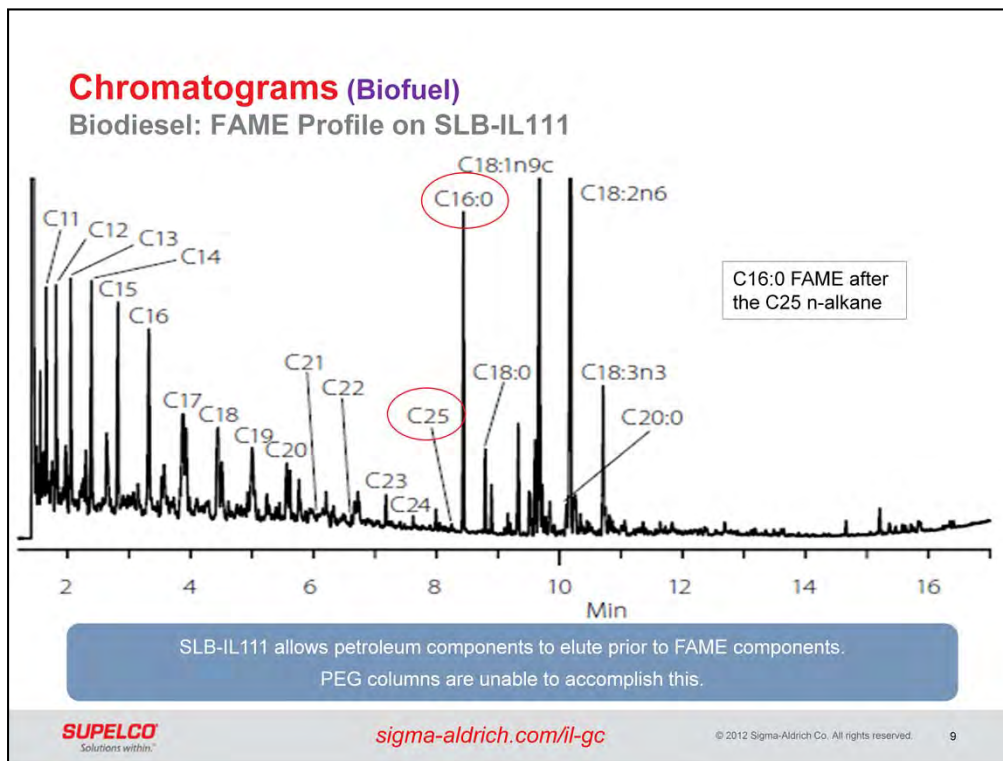
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Chromatograms – Biofuel Applications



B100 biodiesel is 100% biomass-based diesel. It is often blended with petroleum-based diesel before consumer use. A common blend is B20, which is 20% biomass-based diesel and 80% petroleum-based diesel. Once blended, the FAME profile cannot be determined using a polar column with a polyethylene glycol phase. This is because there is overlap between the petroleum-based biodiesel compounds and the biomass-based diesel compounds. Use of the extremely polar SLB-IL111 column allows the FAME profile of blended biodiesel to be determined. This is accomplished by separation of compound classes (aliphatic hydrocarbons from the petroleum-based diesel prior to FAMES from the biomass-based diesel). Shown in this slide is a B20 biodiesel sample. Specifically, the C16:0 FAME (the first major FAME in the sample) elutes after the C25 n-alkane (the last significant n-alkane in the sample).

Conditions

- column: SLB-IL111, 30 m x 0.25 mm I.D., 0.20 μm (28927-U)
- oven: 50 $^{\circ}\text{C}$, 13 $^{\circ}\text{C}/\text{min}$ to 270 $^{\circ}\text{C}$ (5 min)
- inj. temp.: 250 $^{\circ}\text{C}$
- detector: FID, 270 $^{\circ}\text{C}$
- carrier gas: helium, 40 cm/sec
- injection: 1 μL , 100:1 split
- liner: 4 mm I.D., split/splitless type, wool packed FocusLiner design
- sample: B20 biodiesel (soy source) diluted 1:20 in n-hexane

[Chromatogram ID = G005423]

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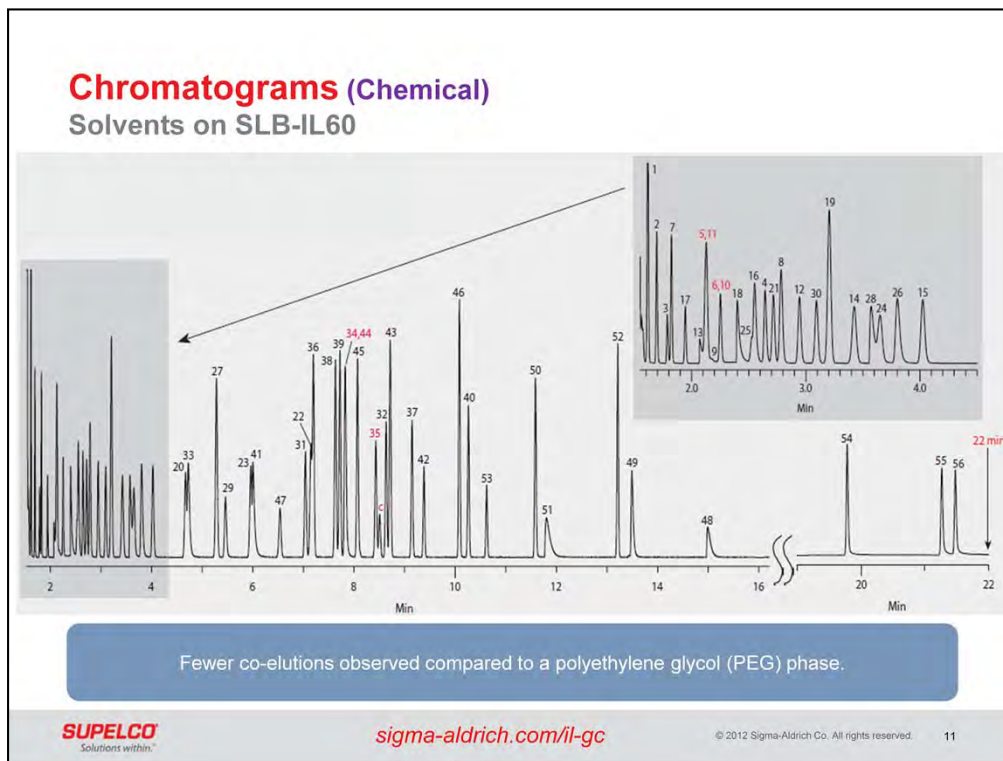
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Chromatograms – Chemical Applications

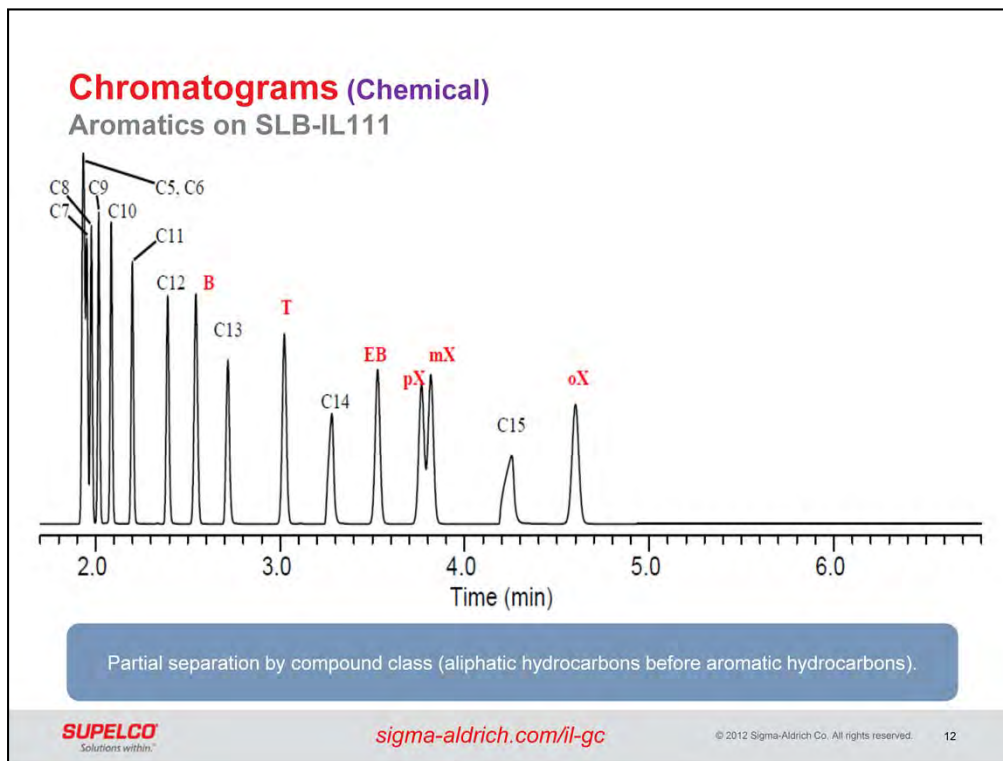


Columns based on polyethylene glycol (PEG) phase chemistry are widely used for a variety of applications, such as industrial solvents. However, it is advantageous to possess columns with alternative selectivity, because resolution can be greatly affected by selectivity. This chromatogram is of a 56-component industrial solvent mix containing alcohols, aldehydes, aromatics, chlorinated hydrocarbons, esters, ethers, ketones, and nitrogen-containing compounds on an SLB-IL60 column. The SLB-IL60 column is not based on a PEG phase. It is made with an ionic liquid phase, and has various functional groups that allow for an increased number of interaction mechanisms compared to a PEG phase. This results in fewer co-elutions compared to those observed on columns made with a PEG phase.

Conditions

- column: SLB-IL60, 30 m x 0.25 mm I.D., 0.20 μm (29505-U)
- oven: 40 $^{\circ}\text{C}$ (4 min), 8 $^{\circ}\text{C}/\text{min}$ to 200 $^{\circ}\text{C}$ (5 min)
- inj. temp.: 250 $^{\circ}\text{C}$
- carrier gas: helium, 30 cm/sec
- detector: FID, 250 $^{\circ}\text{C}$
- injection: 1 μL , 100:1 split
- liner: 4 mm I.D., split/splitless type, wool packed single taper FocusLiner design
- sample: 56-component industrial solvent mix, each analyte at 0.2 % (v/v) in pentane

[Chromatogram ID = G005769]



Aromatic hydrocarbons are widely used starting materials and intermediates in the manufacture of other chemicals, which are then used to make dyes, polyurethanes, plastics, synthetic fibers, and many more products. Aliphatic hydrocarbons may be present as contaminants. This chromatogram of an aromatic/aliphatic hydrocarbon mix was generated using an SLB-IL111 ionic liquid column. The powerful selectivity of this phase for polarizable analytes (contain double and/or triple C-C bonds) is able to produce partial separation by compound class (aliphatic hydrocarbons before aromatic hydrocarbons).

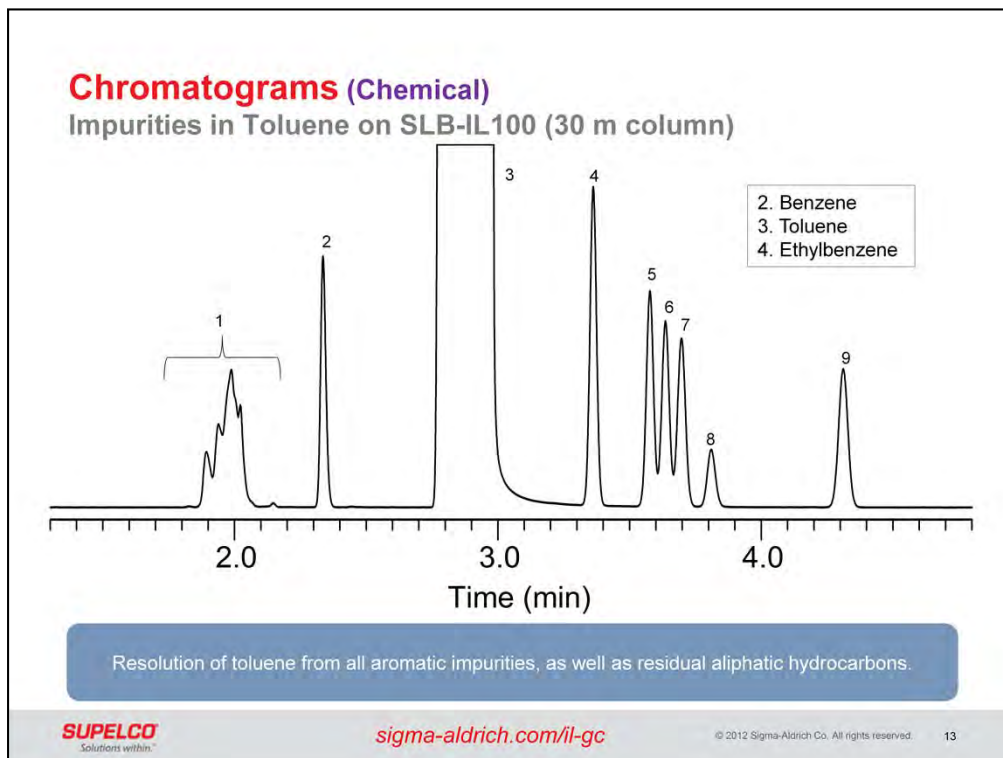
Peak IDs (boiling point order)

- C5 = Pentane
- C6 = Hexane
- B = Benzene
- C7 = Heptane
- T = Toluene
- C8 = Octane
- EB = Ethylbenzene
- pX = p-Xylene
- mX = m-Xylene
- oX = o-Xylene
- C9 = Nonane
- C10 = Decane
- C11 = Undecane
- C12 = Dodecane
- C13 = Tridecane
- C14 = Tetradecane
- C15 = Pentadecane

Conditions

- columns: SLB-IL111, 30 m x 0.25 mm I.D., 0.20 μ m (28927-U)
- oven: 65 °C
- inj. temp.: 250 °C
- detector: FID, 265 °C
- carrier gas: helium, 30 cm/sec
- injection: wet needle, 200:1 split
- liner: 4 mm I.D., split/splitless type, wool packed single taper FocusLiner design
- sample: Neat mixture of C5-C15 n-alkanes + BTEX, equal volumes

[Chromatogram ID = G005317]



Toluene is primarily used as an industrial solvent, but is also the industrial feedstock in the production of TNT. Toluene can contain trace amounts of other aromatics, because these compounds are structurally similar. This chromatogram of a toluene sample was generated using an SLB-IL100 ionic liquid column. The sample was spiked with aromatic impurities at 0.01% to highlight the ability of this column's selectivity to provide resolution of toluene from all aromatic impurities, as well as residual aliphatic hydrocarbons.

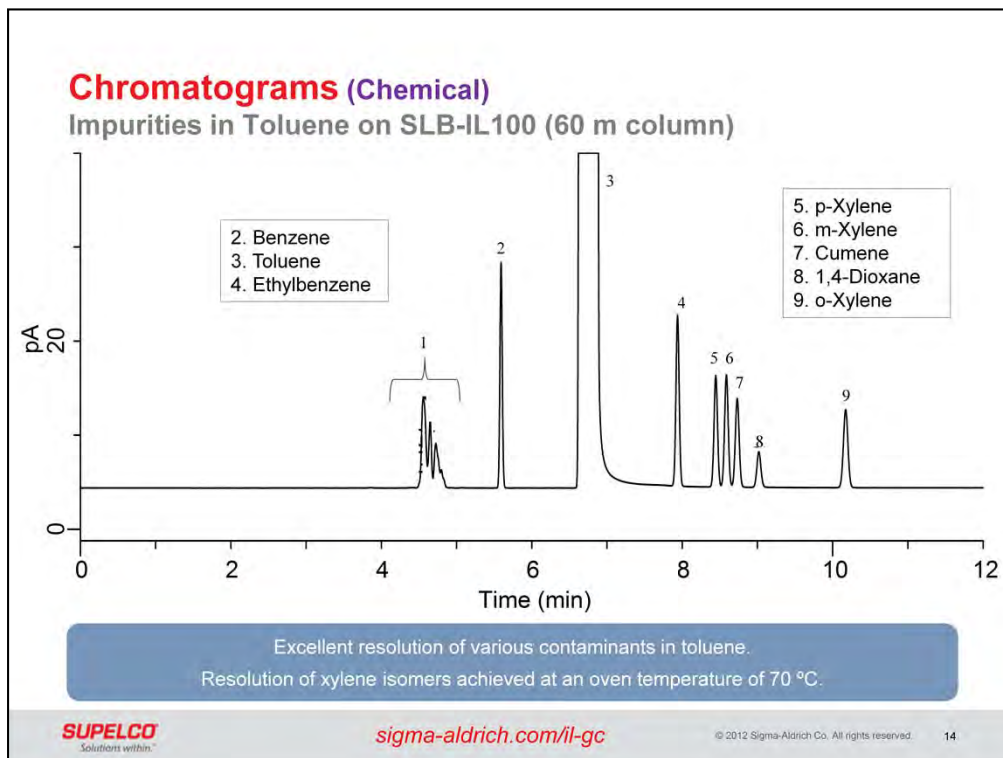
Peak IDs

1. Aliphatic hydrocarbons
2. Benzene
3. Toluene
4. Ethylbenzene
5. p-Xylene
6. m-Xylene
7. Isopropylbenzene (cumene)
8. 1,4-Dioxane
9. o-Xylene

Conditions

- column: SLB-IL100, 30 m x 0.25 mm I.D., 0.20 μ m (28884-U)
- oven: 70 °C
- inj. temp.: 200 °C
- detector: FID, 200 °C
- carrier gas: helium, 28 cm/sec
- injection: 1 μ L, 40:1 split
- liner: 4 mm I.D., split type, cup design
- sample: toluene, with each aromatic impurity spiked at 0.01% by weight

[Chromatogram ID = G006239]



Toluene is primarily used as an industrial solvent, but is also the industrial feedstock in the production of TNT. Toluene can contain trace amounts of other aromatics, because these compounds are structurally similar. This chromatogram of a toluene sample was generated using an SLB-IL100 ionic liquid column. The sample was spiked with aromatic impurities at 0.01% to highlight the ability of this column's selectivity to provide resolution of toluene from all aromatic impurities, as well as residual aliphatic hydrocarbons. The longer 60 m SLB-IL100 column under these conditions can also be used to resolve xylene isomers.

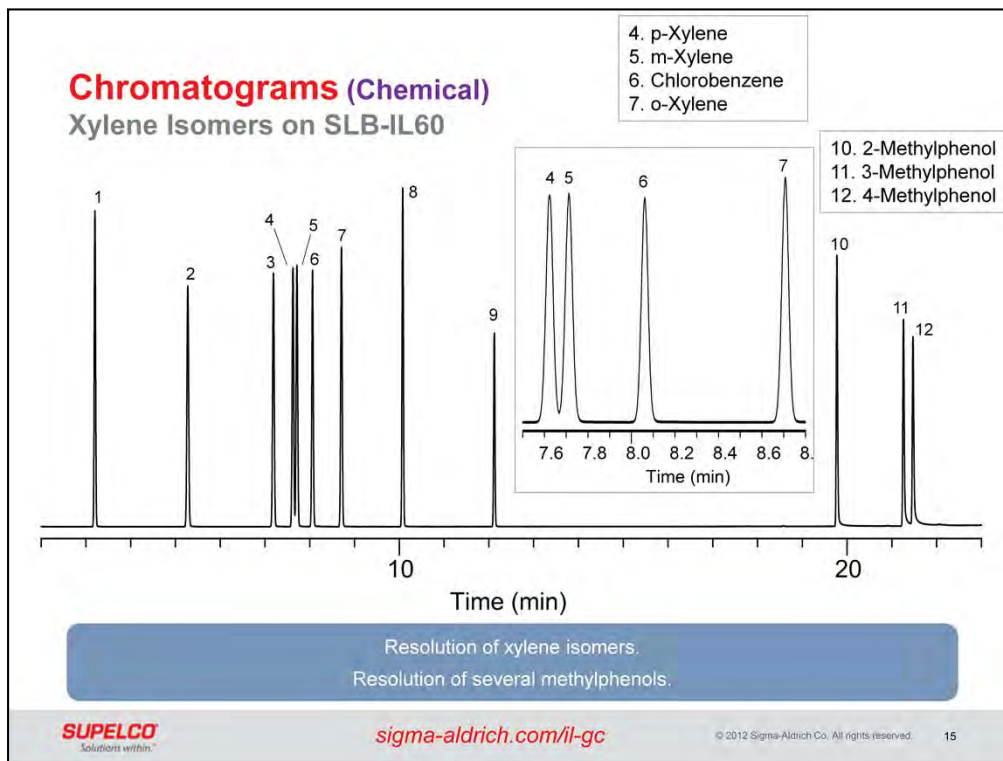
Peak IDs

1. Alkanes
2. Benzene
3. Toluene
4. Ethylbenzene
5. p-Xylene
6. m-Xylene
7. Cumene
8. 1,4-Dioxane
9. o-Xylene

Conditions

- column: SLB-IL100, 60 m x 0.32 mm I.D., 0.20 μ m (28888-U)
- oven: 70 °C
- inj. temp.: 150 °C
- detector: 230 °C
- carrier gas: helium, 25 cm/sec
- injection: 1 μ L, 40:1 split
- sample: toluene spiked with 100 ppm (v/v) of benzene, ethylbenzene, p-xylene, cumene, o-xylene, and dioxane

[Chromatogram ID = G006240]



The xylene isomers are precursors to many chemicals:

- o-xylene is a precursor for phthalic anhydride
- m-xylene is a precursor for isophthalic acid
- p-xylene is a precursor for terephthalic acid and dimethyl terephthalate

The cresol (methylphenol) isomers are also precursors to many chemicals. This chromatogram of a mix of aromatic and methylphenol compounds was generated using an SLB-IL60 ionic liquid column. Its interaction mechanisms allow the separation of all three xylene isomers, and all three cresol isomers.

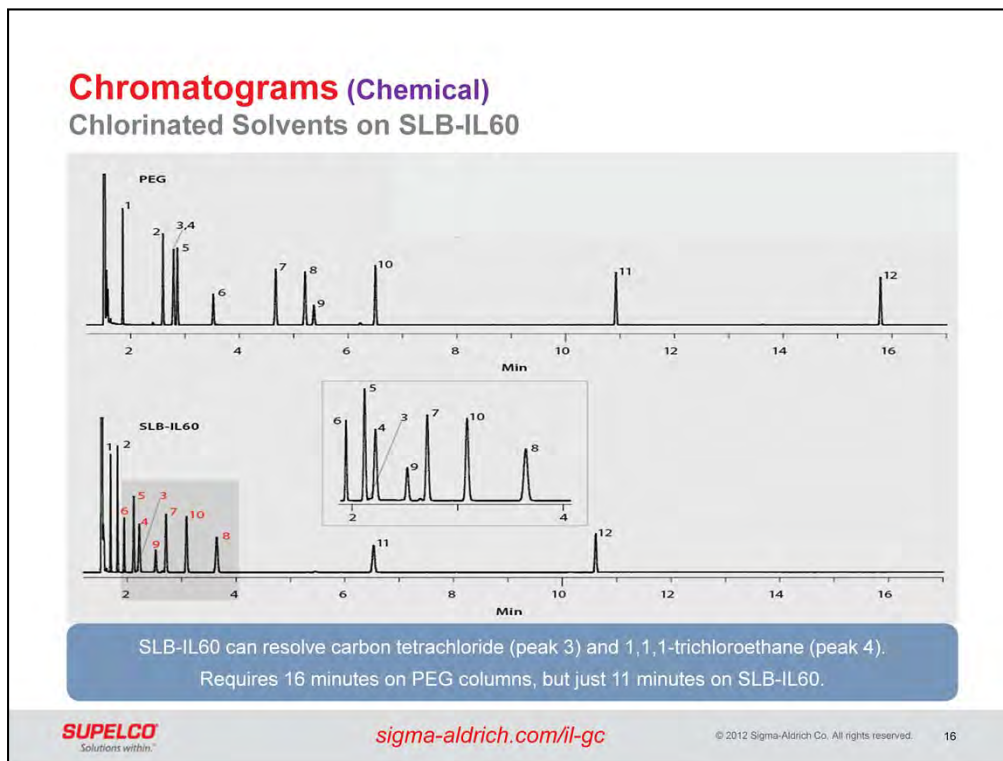
Peaks IDs

1. Benzene
2. Toluene
3. Ethylbenzene
4. p-Xylene
5. m-Xylene
6. Chlorobenzene
7. o-Xylene
8. Styrene
9. 1,4-Dichlorobenzene
10. 2-Methylphenol
11. 3-Methylphenol
12. 4-Methylphenol

Conditions

- column: SLB-IL60, 30 m x 0.25 mm I.D., 0.20 μ m (29505-U)
- oven: 40 $^{\circ}$ C (4 min), 8 $^{\circ}$ C/min to 200 $^{\circ}$ C (5 min)
- inj. temp.: 250 $^{\circ}$ C
- detector: FID, 250 $^{\circ}$ C
- carrier gas: 30 cm/sec constant pressure
- injection: 1 μ L, 100:1 split
- liner: 4 mm I.D., split/splitless type, wool packed single taper FocusLiner design
- sample: 12 analytes, each at 0.2% (v/v) in pentane

[Chromatogram ID = G006241]



Chlorinated hydrocarbons are used in the manufacture of solvents, pesticides, coatings, polymers, and synthetic rubber. This slide compares chromatograms of a 12-component chlorinated hydrocarbon mix generated using a column made with a polyethylene glycol (PEG) phase to an SLB-IL60 ionic liquid column. The SLB-IL60 column has various functional groups that allow for an increased number of interaction mechanisms compared to PEG columns, and results in alternative selectivity. Compared to analysis on a PEG column, the SLB-IL60 provides:

- Many elution order differences (peaks 3-10)
- Resolution of carbon tetrachloride (peak 3) and 1,1,1-trichloroethane (peak 4)
- Quicker analysis time (11 minutes compared to 16 minutes)

Peak IDs

1. 1,1-Dichloroethylene
2. trans-1,2-Dichloroethylene
3. Carbon tetrachloride
4. 1,1,1-Trichloroethane
5. 1,1-Dichloroethane
6. Methylene chloride
7. Trichloroethylene
8. Tetrachloroethene
9. Chloroform
10. 1,2-Dichloroethane
11. 1,1,1,2-Tetrachloroethane
12. 1,1,2,2-Tetrachloroethane

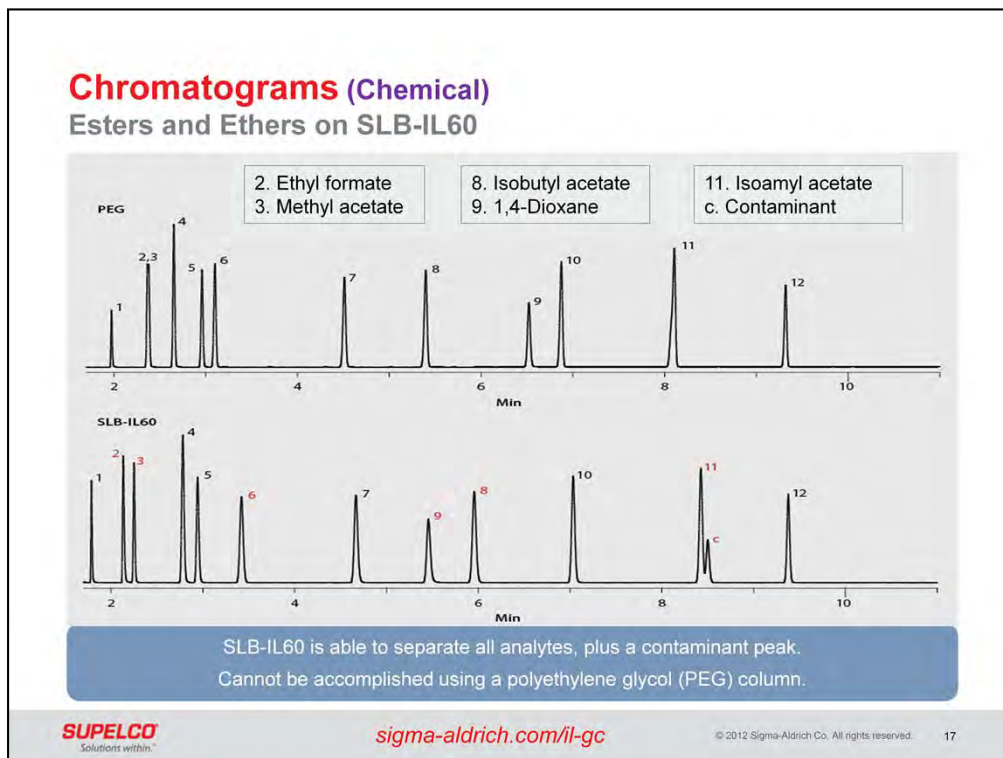
PEG Conditions

- column: PEG, 30 m x 0.25 mm I.D., 0.25 μ m
- oven: 40 $^{\circ}$ C (4 min), 8 $^{\circ}$ C/min to 200 $^{\circ}$ C (5 min)
- inj. temp.: 250 $^{\circ}$ C
- carrier gas: helium, 30 cm/sec
- detector: FID, 250 $^{\circ}$ C
- injection: 1 μ L, 100:1 split
- liner: 4 mm I.D., split/splitless type, wool packed single taper FocusLiner design
- sample: 12-component chlorinated solvent mix, each analyte at 0.2 % (v/v) in pentane

SLB-IL60 Conditions

- column: SLB-IL60, 30 m x 0.25 mm I.D., 0.20 μ m (29505-U)
- All other conditions the same as those used for the PEG

[Chromatogram ID = G006231]



Esters and ethers are also important compound classes used as starting materials in the chemical industry. Esters are refined for use as flavors and fragrances. Ethers are used in the production of downstream products including drugs and industrial solvents. These chromatograms of a 12-component esters and ethers mix were generated using a column made with a polyethylene glycol (PEG) phase and an SLB-IL60 ionic liquid column. Compared to analysis on the PEG column, the SLB-IL60 provides:

- Resolution of ethyl formate (peak 2) and methyl acetate (peak 3)
- Improved resolution of isopropyl acetate (peak 6) from ethyl acetate (peak 5)
- Elution order change for isobutyl acetate (peak 8) and 1,4-dioxane (peak 9)
- Partial resolution of isoamyl acetate (peak 11) from a contaminant peak (peak c), suspected to be 2-methylbutyl acetate [no resolution obtained on PEG columns]

Peaks IDs

1. Methyl formate
2. Ethyl formate
3. Methyl acetate
4. Tetrahydrofuran
5. Ethyl acetate
6. Isopropyl acetate
7. n-Propyl acetate
8. Isobutyl acetate
9. 1,4-Dioxane
10. n-Butyl acetate
11. Isoamyl acetate
12. n-Amyl acetate
- c. Contaminant (2-Methylbutyl acetate?)

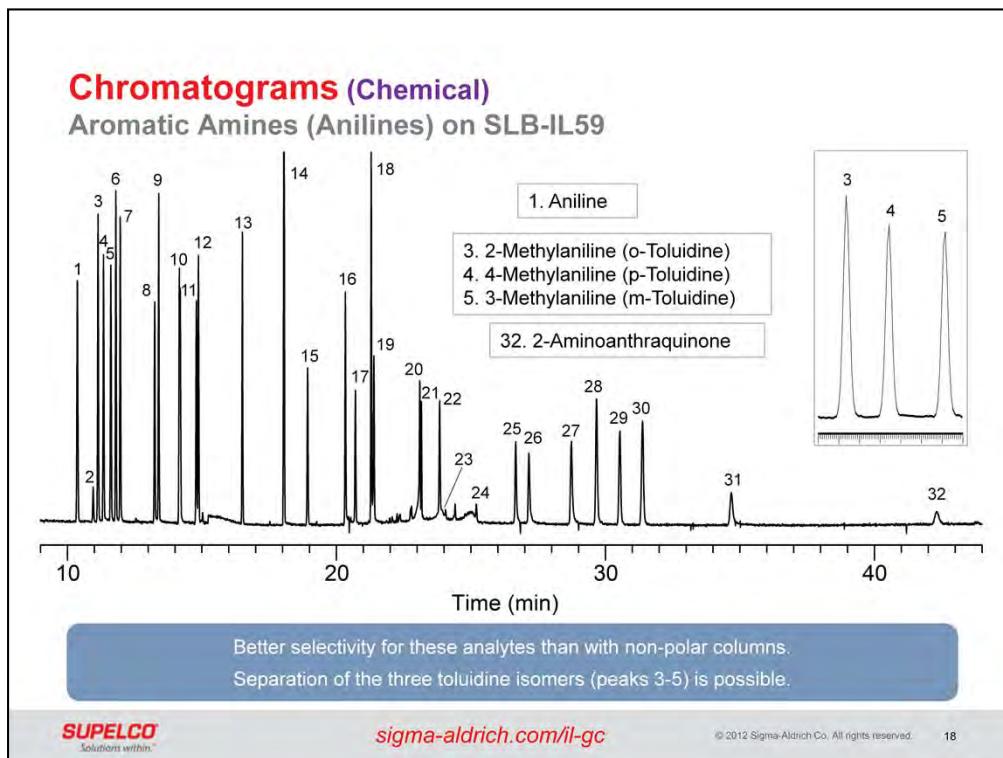
PEG Conditions

- column: PEG, 30 m x 0.25 mm I.D., 0.25 μ m
- oven: 40 °C (4 min), 8 °C/min to 200 °C (5 min)
- inj. temp.: 250 °C
- carrier gas: helium, 30 cm/sec
- detector: FID, 250 °C
- injection: 1 μ L, 100:1 split
- liner: 4 mm I.D., split/splitless type, wool packed single taper FocusLiner design
- sample: 12-component esters and ethers mix, each analyte at 0.2 % (v/v) in pentane

SLB-IL60 Conditions

- column: SLB-IL60, 30 m x 0.25 mm I.D., 0.20 μ m (29505-U)
- All other conditions the same as those used for the PEG

[Chromatogram ID = G006230]

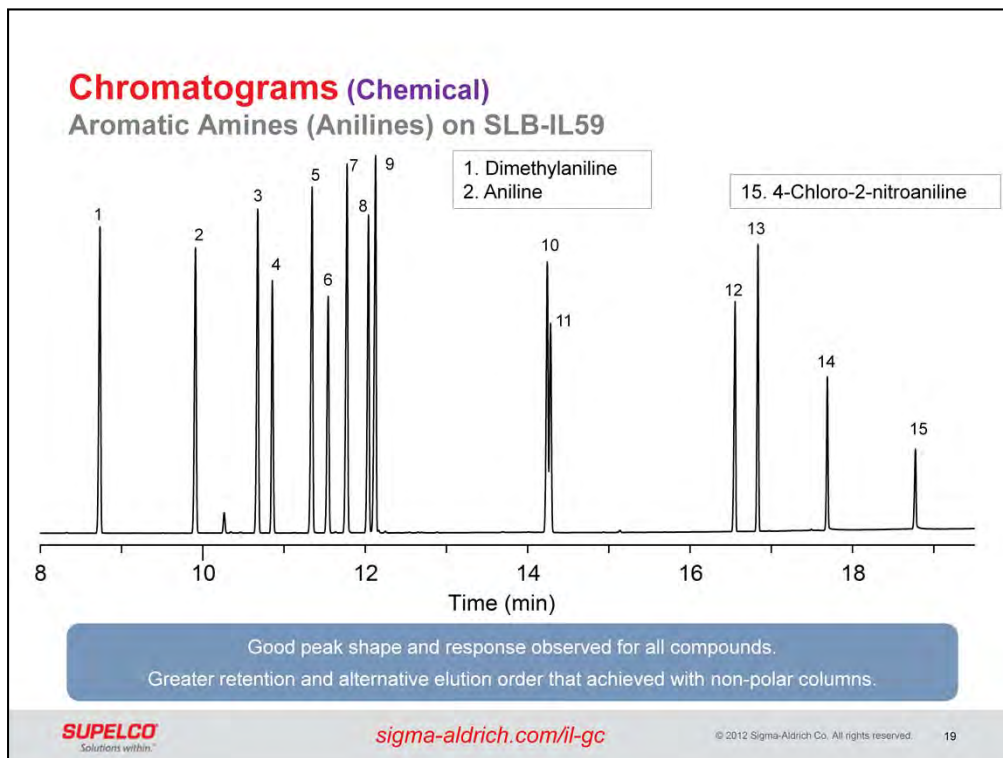


Aromatic amines are used in the production of azo dyes which are then used in textiles and hair coloring. They are also used to make products such as pesticides and basic drugs. This chromatogram of an aromatic amines mix was generated using an SLB-IL59 ionic liquid column with MS detection. This column offers better selectivity for these analytes compared to a non-polar column, and has better stability and a higher operating temperature compared to polar columns made with a polyethylene glycol (PEG) phase. Analytes range from aniline (peak 1) to 2-aminoanthraquinone (peak 32). Separation of the three toluidine isomers (peaks 3-5) is possible.

Conditions

- column: SLB-IL59, 30 m x 0.25 mm I.D., 0.20 μm (28891-U)
- oven: 75 $^{\circ}\text{C}$ (2 min), 10 $^{\circ}\text{C}/\text{min}$ to 250 $^{\circ}\text{C}$, 15 $^{\circ}\text{C}/\text{min}$ to 300 $^{\circ}\text{C}$ (25 min)
- inj. temp.: 250 $^{\circ}\text{C}$
- detector: MSD, interface 275 $^{\circ}\text{C}$, $m/z = 30-300$
- carrier gas: helium, 0.7 mL/min constant
- injection: 1.0 μL , pulsed splitless (25 psi pulse)
- liner: 4 mm I.D., split/splitless type, single taper design
- sample: Each analyte at 50 $\mu\text{g}/\text{mL}$ in methylene chloride

[Chromatogram ID = G006243]



This chromatogram of an aromatic amines mix was generated using an SLB-IL59 ionic liquid column with FID detection. Analytes range in size from aniline (peak 2) to 4-chloro-2-nitroaniline (peak 15). Good peak shape and response was observed for all compounds. Compared to a non-polar column, retention of analytes was greater, and elution order was markedly different.

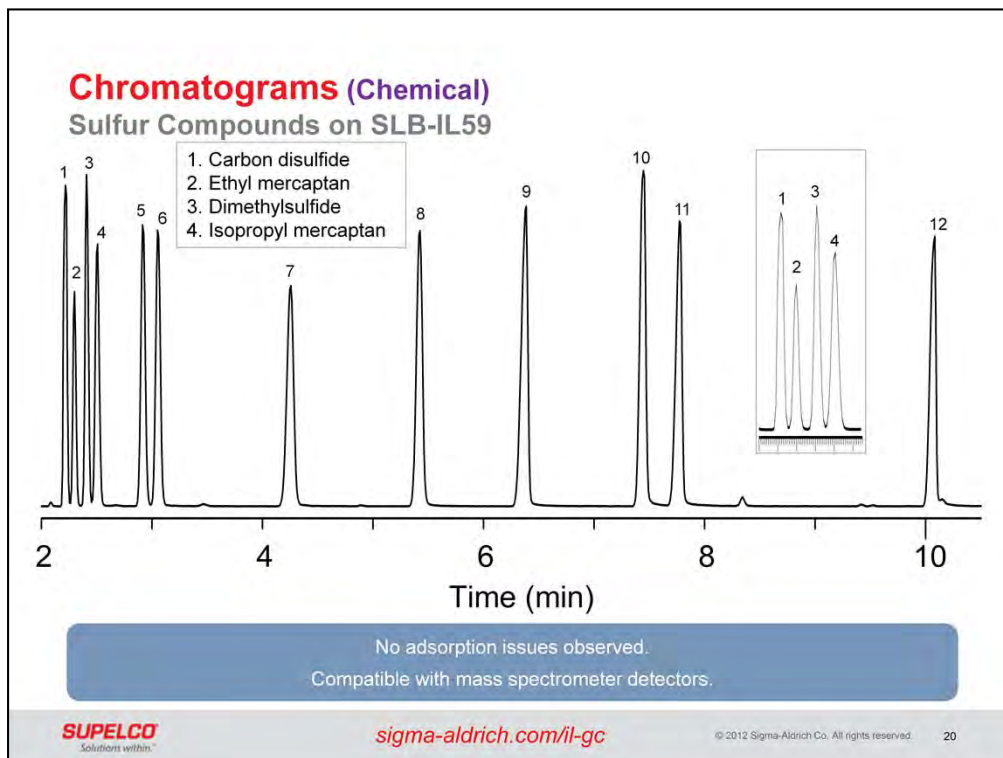
Peak IDs

1. Dimethylaniline
2. Aniline
3. o-Toluidine
4. 3-Aminobenzotrifluoride
5. 2,6-Dimethylaniline
6. 2-Chloroaniline
7. 4-Isopropylaniline
8. 2-Methyl-6-ethylaniline
9. 2,6-Diethylaniline
10. 3-Chloro-4-methylaniline
11. 3-Chloro-4-fluoroaniline
12. 2,4,5-Trichloroaniline
13. 3,4-Dichloroaniline
14. 2,4-Diaminotoluene
15. 4-Chloro-2-nitroaniline

Conditions

- column: SLB-IL59, 30 m x 0.25 mm I.D., 0.20 μ m (28891-U)
- oven: 75 $^{\circ}$ C, (2 min) 10 $^{\circ}$ C/min to 200 $^{\circ}$ C, 20 $^{\circ}$ C/min to 300 $^{\circ}$ C (10 min)
- inj. temp.: 250 $^{\circ}$ C
- detector: FID, 300 $^{\circ}$ C
- carrier gas: helium, 1.5 mL/min constant
- injection: 0.5 μ L, 100:1 split
- liner: 4 mm I.D., split/splitless type, single taper design
- sample: Each analyte at 5000 μ g/mL in methylene chloride

[Chromatogram ID = G006242]



Ionic liquid columns can also be used for the analysis of sulfur compounds. This chromatogram shows the analysis of 12 sulfur compounds on the SLB-IL59 column using a mass spectrometer for detection. Analytes include carbon disulfide (peak 1) to diethyl disulfide (peak 12). No adsorption issues were observed. The inset shows the separation of the first four analytes.

Peak IDs

1. Carbon disulfide
2. Ethyl mercaptan
3. Dimethylsulfide
4. Isopropyl mercaptan
5. n-Propyl mercaptan
6. Ethyl methyl sulfide
7. Diethyl sulfide
8. Thiophene
9. Dimethyl disulfide
10. 2-Methyl thiophene
11. Thiophane
12. Diethyl disulfide

Conditions

- column: SLB-IL59, 30 m x 0.25 mm I.D., 0.20 μ m (28891-U)
- oven: 30 $^{\circ}$ C (4 min), 10 $^{\circ}$ C/min to 300 $^{\circ}$ C
- inj. temp.: 250 $^{\circ}$ C
- detector: MSD, interface at 275 $^{\circ}$ C
- carrier gas: helium, 30 cm/sec constant
- injection: 0.2 μ L, split 100:1
- liner: 4 mm I.D., split/splitless type, dual taper design
- sample: 12 sulfur compounds, neat mix

[Chromatogram ID = G006244]

Agenda

- Chromatograms
- Summary / Related Products / Resources

- Environmental
- Petroleum
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- Chemical
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- Food and Beverage
- Flavor and Fragrance
- Clinical
- General Analytical

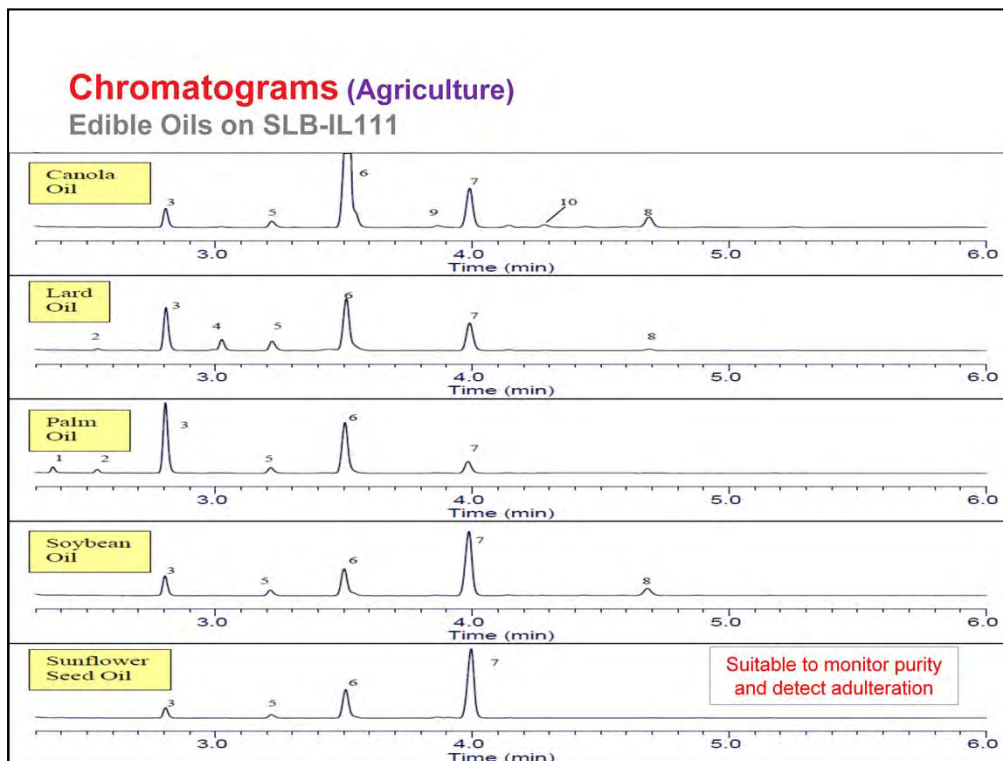
Analyte IDs and GC conditions are included in the speaker notes for most chromatograms. Otherwise, enter chromatogram ID from speaker notes into the search bar at <sigma-aldrich.com>.

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Chromatograms – Agriculture Applications



Each pure edible oil has a unique combination of FAMES in specific ratios. Therefore, GC fingerprinting can be used to monitor purity. It can also be used to detect adulteration when a cheaper, inferior oil is added to boost the volume of a premium, higher priced oil. The SLB-IL111 column is able to provide the necessary resolution of key FAME isomers found in several edible oils for effective fingerprinting.

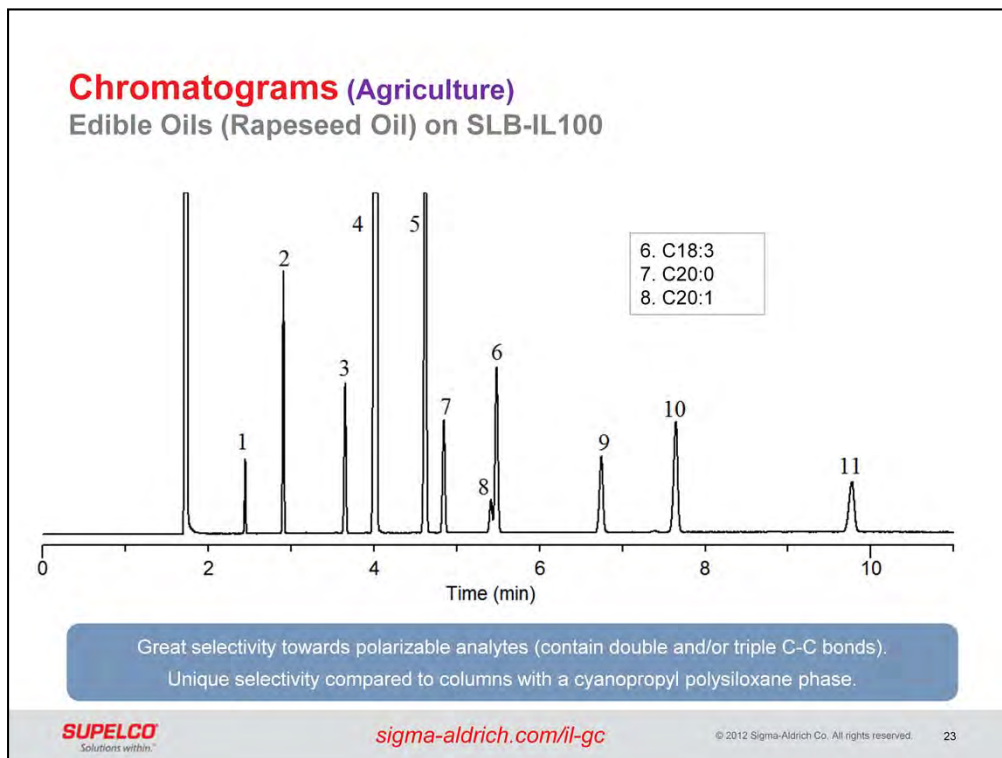
Peak IDs

1. Lauric acid methyl ester (C12:0)
2. Myristic acid methyl ester (C14:0)
3. Palmitic acid methyl ester (C16:0)
4. Palmitoleic acid methyl ester (C16:1)
5. Stearic acid methyl ester (C18:0)
6. Oleic acid methyl ester (C18:1n9c)
7. Linoleic acid methyl ester (C18:2n6c)
8. Linolenic acid methyl ester (C18:3n3)
9. Arachidic acid methyl ester (C20:0)
10. cis-11-Eicosenoic acid methyl ester (C20:1)

Conditions

- column: SLB-IL111, 30 m x 0.25 mm I.D., 0.20 μ m (28927-U)
- oven: 180 $^{\circ}$ C
- inj. temp.: 250 $^{\circ}$ C
- detector: FID, 260 $^{\circ}$ C
- carrier gas: helium, 25 cm/sec
- injection: 1 μ L, 50:1 split
- liner: 4 mm I.D., split type, cup design

[Chromatogram ID = G005480]



Rapeseed oil is a simple vegetable oil that contains a series of saturated and unsaturated fatty acids ranging from C14 through C24 in carbon number. Monitoring the elution locations of C18:3 (peak 6), C20:0 (peak 7), and C20:1 (peak 8) relative to each other, as well as the other FAMES, is an indication of a column's relative strength of dipole-induced dipole interactions. The SLB-IL100 column has great selectivity towards polarizable analytes (contain double and/or triple C-C bonds). It provides a unique selectivity compared to columns with a cyanopropyl polysiloxane phase.

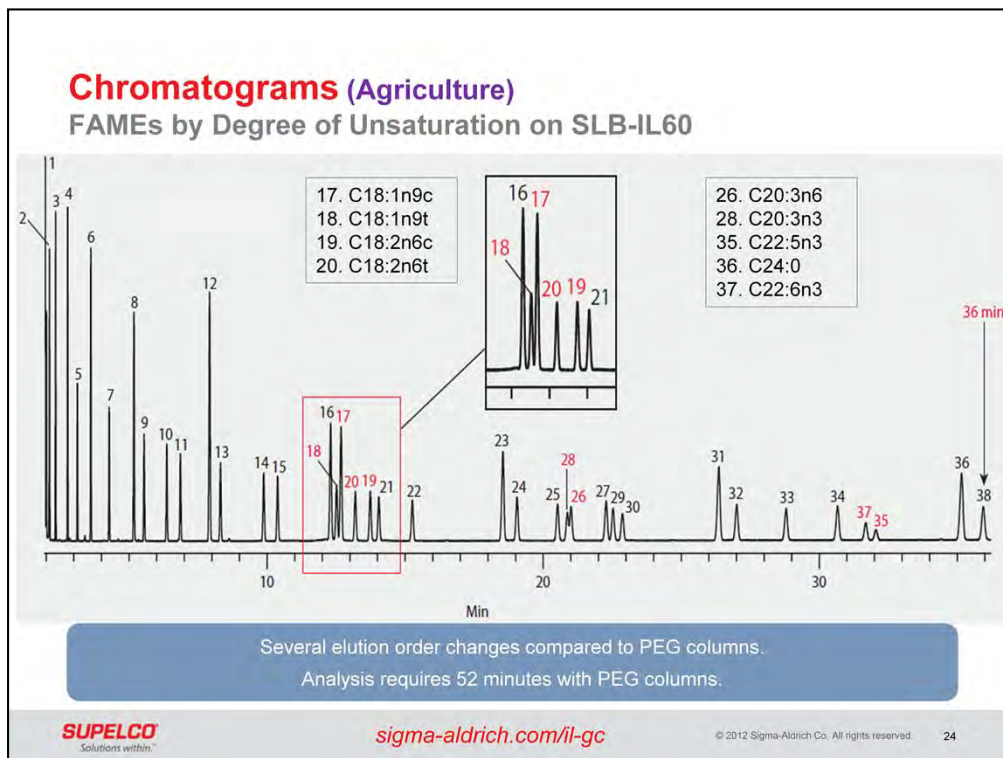
Peak IDs

1. Myristic (C14:0)
2. Palmitic (C16:0)
3. Stearic (C18:0)
4. Oleic (C18:1n9c)
5. Linoleic (C18:2)
6. Linolenic (C18:3)
7. Arachidic (C20:0)
8. cis-11-Eicosenoic (C20:1)
9. Behenic (C22:0)
10. Erucic (C22:1)
11. Lignoceric (C24:0)

Conditions

- column: SLB-IL100, 30 m x 0.25 mm I.D., 0.20 μ m (28884-U)
- oven: 180 $^{\circ}$ C
- inj. temp.: 250 $^{\circ}$ C
- detector: FID, 250 $^{\circ}$ C
- carrier gas: helium, 30 cm/sec @ 180 $^{\circ}$ C
- injection: 1 μ L, 100:1 split
- liner: 4 mm I.D., split type, cup design
- sample: Rapeseed oil FAME mix, 5 mg/mL total FAMES in methylene chloride

[Chromatogram ID = G004218]

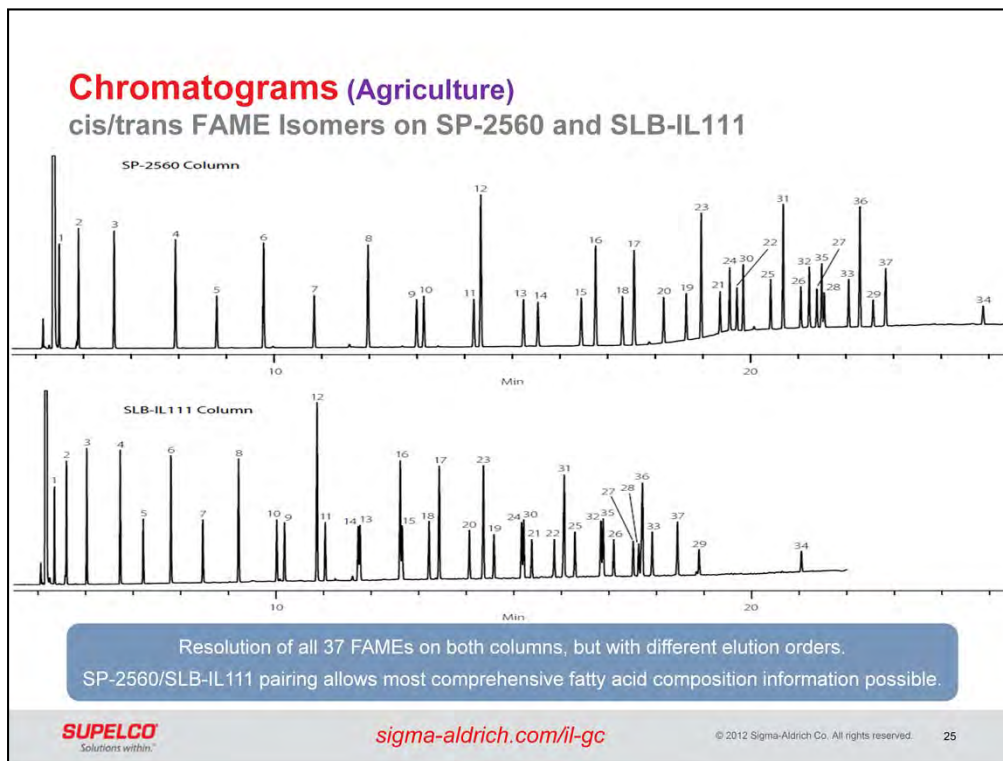


Analyzing FAMES by degree of unsaturation is used to determine the amount of saturated, monounsaturated, and polyunsaturated fats. This chromatogram of C4 to C24 FAMES was analyzed on the SLB-IL60 column. Some interesting elution order changes were noted between the SLB-IL60 and columns made with a polyethylene glycol (PEG) phase. Especially surprising was the elution of C22:6n3 (peak 37) before C22:5n3 (peak 35). Even with one more double bond, it exhibited less retention. Also of note is that this analysis requires 52 minutes with a PEG column. The SLB-IL60 is able to perform this in just 36 minutes.

Conditions

- column: SLB-IL60, 30 m x 0.25 mm I.D., 0.20 μ m (29505-U)
- oven: 170 $^{\circ}$ C, 1 $^{\circ}$ C/min to 225 $^{\circ}$ C
- inj. temp.: 250 $^{\circ}$ C
- detector: FID, 260 $^{\circ}$ C
- carrier gas: helium, 1.2 mL/min
- injection: 1 μ L, 100:1 split
- liner: 4 mm I.D., split/splitless type, single taper wool packed FocusLiner design
- sample: Supelco 37-Component FAME Mix (47885-U) + C22:5n3, in methylene chloride

[Chromatogram ID = G005763]



Trans fat content is reported on nutritional facts panels as part of proper food labeling. It is desirable to use a column which can resolve trans FAME isomers from cis FAME isomers, so trans fat values are not biased high. These chromatograms of C4 to C24 FAMEs on the SP-2560 and SLB-IL111 represent the ultimate in cis/trans FAME analysis. This is because the SP-2560/SLB-IL111 pairing allows the most comprehensive fatty acid composition information possible.

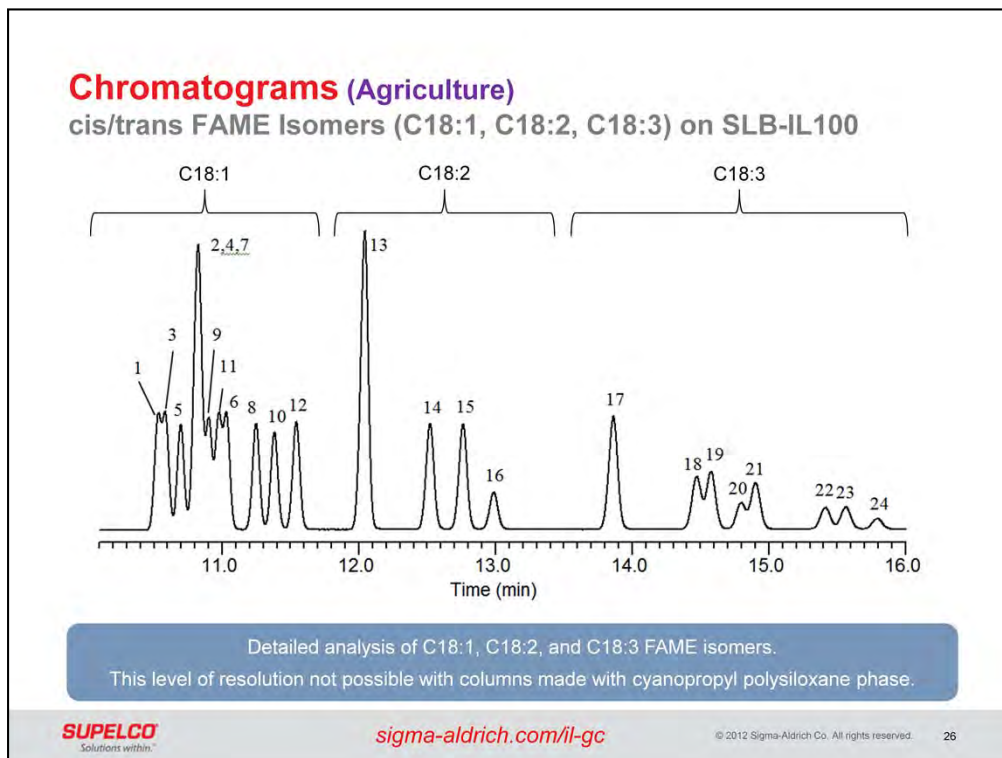
SP-2560 Conditions

- column: SP-2560, 100 m x 0.25 mm I.D., 0.20 μm (24056)
- oven: 140 $^{\circ}\text{C}$ (5 min), 8 $^{\circ}\text{C}/\text{min}$ to 180 $^{\circ}\text{C}$, 4 $^{\circ}\text{C}/\text{min}$ to 210 $^{\circ}\text{C}$, 20 $^{\circ}\text{C}/\text{min}$ to 250 $^{\circ}\text{C}$ (7 min)
- inj. temp.: 250 $^{\circ}\text{C}$
- detector: FID, 250 $^{\circ}\text{C}$
- carrier gas: hydrogen, 40 cm/sec
- injection: 1 μL , 100:1 split
- liner: 4 mm I.D., split type, cup design
- sample: Supelco 37-Component FAME Mix (47885-U)

SLB-IL111 Conditions

- column: SLB-IL111, 100 m x 0.25 mm I.D., 0.20 μm (29647-U)
- oven: 140 $^{\circ}\text{C}$ (5 min), 8 $^{\circ}\text{C}/\text{min}$ to 180 $^{\circ}\text{C}$, 5 $^{\circ}\text{C}/\text{min}$ to 260 $^{\circ}\text{C}$
- detector: FID, 260 $^{\circ}\text{C}$
- All other conditions the same as those used for the SP-2560

[Chromatogram IDs = G005366 (SP-2560), G005367 (SLB-IL111)]



Many regulatory agencies require content labeling to inform buyers of 'trans fat' levels of foods and some dietary supplements. This is because trans fatty acids have adverse health consequences and no known nutritional benefits over other fats. Some of the most common unsaturated fatty acids are the C18 series. This chromatogram shows a detailed analysis of C18:1, C18:2, and C18:3 fatty acid isomers, as fatty acid methyl esters (FAMES), on a SLB-IL100. This level of resolution is not possible with columns made with cyanopropyl polysiloxane phase.

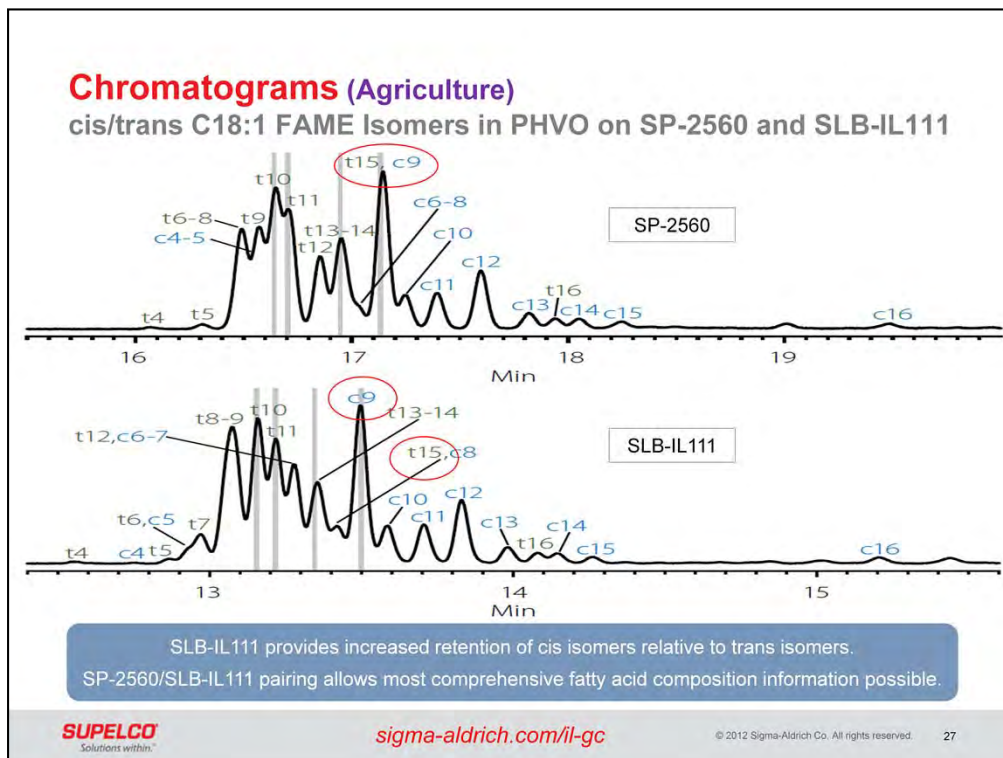
Peak IDs

1. C18:1Δ6t
2. C18:1Δ6c
3. C18:1Δ7t
4. C18:1Δ7c
5. C18:1Δ9t
6. C18:1Δ9c
7. C18:1Δ11t
8. C18:1Δ11c
9. C18:1Δ12t
10. C18:1Δ12c
11. C18:1Δ13t
12. C18:1Δ13c
13. C18:2Δ9t,12t
14. C18:2Δ9c,12t
15. C18:2Δ9t,12c
16. C18:2Δ9c,12c
17. C18:3Δ9t,12t,15t
18. C18:3Δ9t,12t,15c
19. C18:3Δ9t,12c,15t
20. C18:3Δ9c,12c,15t
21. C18:3Δ9c,12t,15t
22. C18:3Δ9c,12t,15c
23. C18:3Δ9t,12c,15c
24. C18:3Δ9c,12c,15c

Conditions

- column: SLB-IL100, 60 m x 0.25 mm I.D., 0.20 μm (28886-U)
- oven: 170 °C
- inj. temp.: 250 °C
- detector: FID, 250 °C
- carrier gas: helium, 30 cm/sec
- injection: 1 μL, 50:1 split
- liner: 4 mm I.D., split type, cup design
- sample: mixture of C18:1, C18:2, and C18:3 FAMES in methylene chloride

[Chromatogram ID = G004386]



Columns made with cyanopropyl polysiloxane phases are traditionally used for the separation of cis and trans geometric positional isomers of fatty acids methyl esters (FAMES). The 100 m SP-2560 column is a workhorse for this application. This slide shows chromatograms of a partially hydrogenated vegetable oil (PHVO) sample run on the 100 m SP-2560 and the 100 m SLB-IL111. When comparing FAME isomers with the same degree of unsaturation, the SLB-IL111 provides increased retention of cis isomers relative to trans isomers with the double bond at the same location. The SLB-IL111 was able to provide resolution of C18:1n9c from C18:1n15t, a separation not possible with the SP-2560. The SLB-IL111 offered improved resolution of some isomers that cannot be completely resolved with the SP-2560 either.

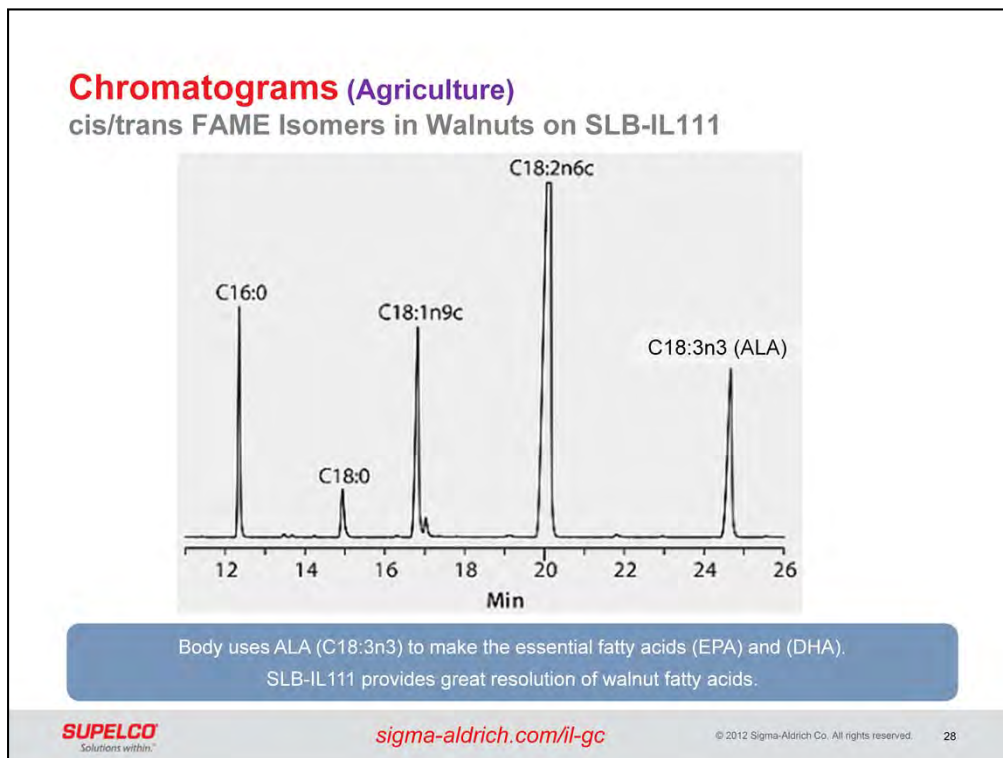
SP-2560 Conditions

- column: SP-2560, 100 m x 0.25 mm I.D., 0.20 μ m (24056)
- oven: 180 $^{\circ}$ C isothermal
- inj. temp: 250 $^{\circ}$ C
- detector: FID, 250 $^{\circ}$ C
- carrier gas: hydrogen, 1 mL/min
- injection: 1 μ L, 100:1 split
- liner: 4 mm I.D., split liner with cup (2051001)

SLB-IL111 Conditions

- column: SLB-IL111, 100 m x 0.25 mm I.D., 0.20 μ m (29647-U)
- oven: 168 $^{\circ}$ C isothermal
- All other conditions the same as those used for the SP-2560

[Chromatogram IDs = G005287 (SP-2560), G005290 (SLB-IL111)]



Nuts are considered nutrient dense foods and their consumption has been associated with a reduced risk of coronary heart disease. The health benefits of nuts are partially attributable to their high content of unsaturated fatty acids. For example, alpha-linolenic acid (ALA), an unsaturated fatty acid found in flaxseeds and walnuts, is a precursor to the formation within the body of the essential fatty acids eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA). This application illustrates the GC analysis of fatty acids extracted from walnuts, considered a significant plant source of (ALA). The SLB-IL111 provides great resolution.

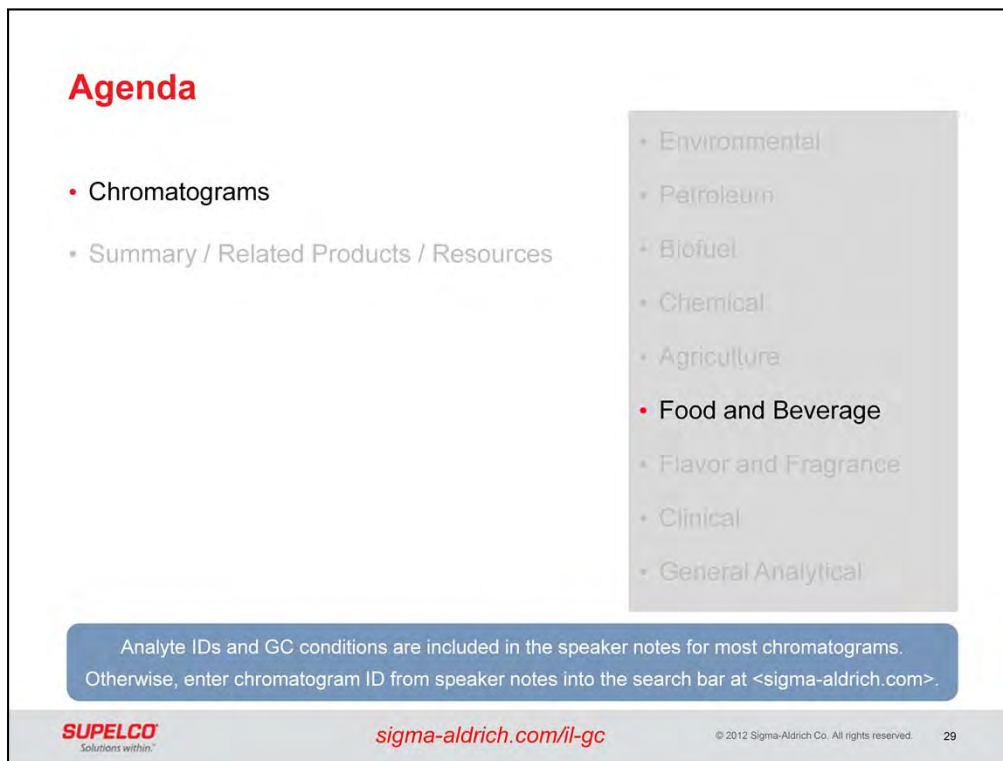
Peak IDs

1. Palmitic acid methyl ester (C16:0)
2. Stearic acid methyl ester (C18:0)
3. Oleic acid methyl ester (C18:1n9c)
4. Linoleic acid methyl ester (C18:2n6c) [LA]
5. alpha-Linolenic acid methyl ester (C18:3n3) [ALA]

Conditions

- column: SLB-IL111, 100 m x 0.25 mm I.D., 0.20 μ m (29647-U)
- oven: 168 °C isothermal
- inj. temp.: 250 °C
- detector: FID, 260 °C
- carrier gas: helium, 1.0 mL/min
- injection: 1 μ L, 100:1 split
- liner: 4 mm I.D., split/splitless type, wool packed single taper FocusLiner design
- sample: extract of walnuts

[Chromatogram IDs = G005823]



Agenda

- Chromatograms
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- Flavor and Fragrance
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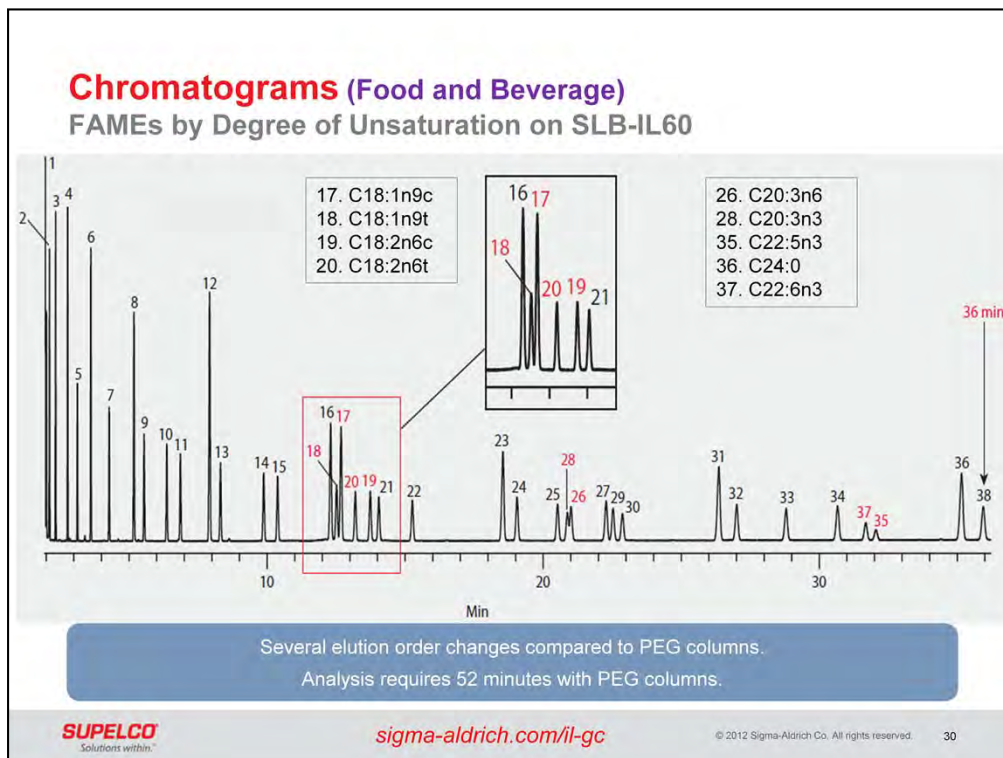
Analyte IDs and GC conditions are included in the speaker notes for most chromatograms. Otherwise, enter chromatogram ID from speaker notes into the search bar at <sigma-aldrich.com>.

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Chromatograms – Food and Beverage Applications

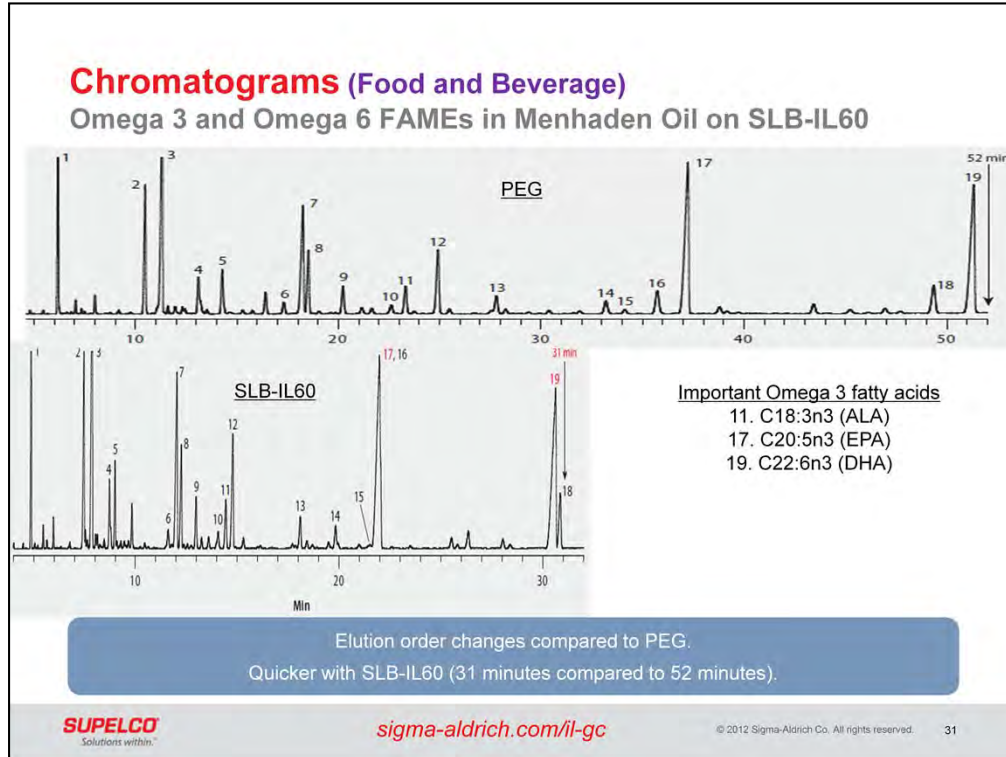


Analyzing FAMES by degree of unsaturation is used to determine the amount of saturated, monounsaturated, and polyunsaturated fats. This chromatogram of C4 to C24 FAMES was analyzed on the SLB-IL60 column. Some interesting elution order changes were noted between the SLB-IL60 and columns made with a polyethylene glycol (PEG) phase. Especially surprising was the elution of C22:6n3 (peak 37) before C22:5n3 (peak 35). Even with one more double bond, it exhibited less retention. Also of note is that this analysis requires 52 minutes with a PEG column. The SLB-IL60 is able to perform this in just 36 minutes.

Conditions

- column: SLB-IL60, 30 m x 0.25 mm I.D., 0.20 μm (29505-U)
- oven: 170 $^{\circ}\text{C}$, 1 $^{\circ}\text{C}/\text{min}$ to 225 $^{\circ}\text{C}$
- inj. temp.: 250 $^{\circ}\text{C}$
- detector: FID, 260 $^{\circ}\text{C}$
- carrier gas: helium, 1.2 mL/min
- injection: 1 μL , 100:1 split
- liner: 4 mm I.D., split/splitless type, single taper wool packed FocusLiner design
- sample: Supelco 37-Component FAME Mix (47885-U) + C22:5n3, in methylene chloride

[Chromatogram ID = G005763]



Menhaden oil contains an abundance of omega 3 fatty acids. This slide compares chromatograms from a column made with polyethylene glycol (PEG) phase to an SLB-IL60. The SLB-IL60 analysis resulted in two elution order changes. Additionally, the analysis was quicker (31 minutes compared to 52 minutes).

Peak IDs

1. C14:0
2. C16:0
3. C16:1n7
4. C16:2n4
5. C16:3n4
6. C18:0
7. C18:1n9
8. C18:1n7
9. C18:2n6
10. C18:3n4
11. C18:3n3 (ALA)
12. C18:4n3
13. C20:1n9
14. C20:3n3
15. C20:4n6
16. C20:4n3
17. C20:5n3 (EPA)
18. C22:5n3
19. C22:6n3 (DHA)

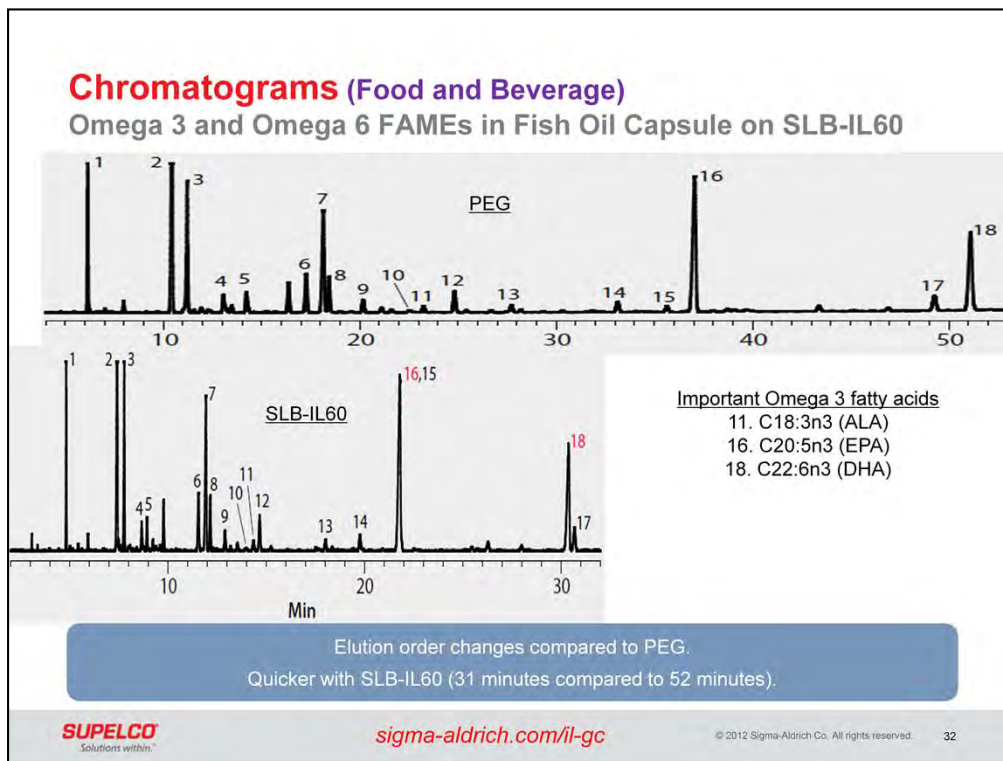
PEG Conditions

- column: Omegawax, 30 m x 0.25 mm I.D., 0.25 µm (24136)
- oven: 170 °C, 1 °C/min to 225 °C
- inj. temp.: 250 °C
- carrier gas: helium, 1.2 mL/min
- detector: FID, 260 °C
- injection: 1 µL, 100:1 split
- liner: 4 mm I.D., split/splitless type, single taper wool packed FocusLiner design
- sample: PUFA No. 3 Mix (47085-U), diluted in 1 mL of hexane

SLB-IL60 Conditions

- column: SLB-IL60, 30 m x 0.25 mm I.D., 0.20 µm (29505-U)
- All other conditions the same as those used for the Omegawax

[Chromatogram IDs = G_____ (Omegawax), G006246 (SLB-IL60)]



Fish oil capsules are taken to gain the benefits associated with omega 3 fatty acids. This sample is very similar to the menhaden oil sample shown on the previous slide. Shown are chromatograms generate with a column made with polyethylene glycol (PEG) phase and an SLB-IL60. The SLB-IL60 analysis resulted in two elution order changes. Additionally, the analysis was quicker (31 minutes compared to 52 minutes).

Peak IDs

1. C14:0
2. C16:0
3. C16:1n7
4. C16:2n4
5. C16:3n4
6. C18:0
7. C18:1n9
8. C18:1n7
9. C18:2n6
10. C18:3n4
11. C18:3n3 (ALA)
12. C18:4n3
13. C20:1n9
14. C20:3n3
15. C20:4n3
16. C20:5n3 (EPA)
17. C22:5n3
18. C22:6n3 (DHA)

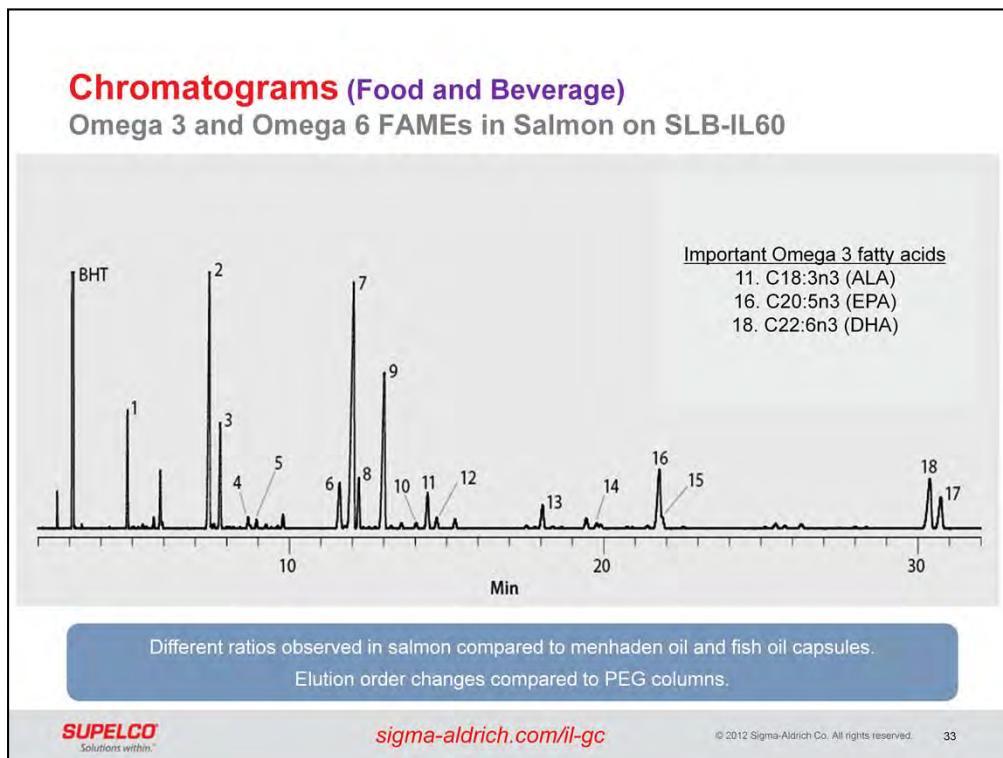
PEG Conditions

- column: Omegawax, 30 m x 0.25 mm I.D., 0.25 μ m (24136)
- oven: 170 $^{\circ}$ C, 1 $^{\circ}$ C/min to 225 $^{\circ}$ C
- inj. temp.: 250 $^{\circ}$ C
- detector: FID, 260 $^{\circ}$ C
- carrier gas: helium, 1.2 mL/min
- injection: 1 μ L, 100:1 split
- liner: 4 mm I.D., split/splitless type, wool packed single taper FocusLiner design

SLB-IL60 Conditions

- column: SLB-IL60, 30 m x 0.25 mm I.D., 0.20 μ m (29505-U)
- All other conditions the same as those used for the Omegawax

[Chromatogram IDs = G005813 (Omegawax), G006247 (SLB-IL60)]



This chromatogram shows analysis on the SLB-IL60 of a farm-raised Atlantic salmon purchased at a local grocery store. Extraction was performed using AOCS Official Method Ce 1k-09, with BHT added as an antioxidant. The fatty acids found were as expected based on the literature. Of note is the different ratios observed in the salmon compared to the menhaden oil and fish oil capsule chromatograms on previous slides. Analysis on the SLB-IL60 was characterized by two elution order changes from what is observed on PEG columns.

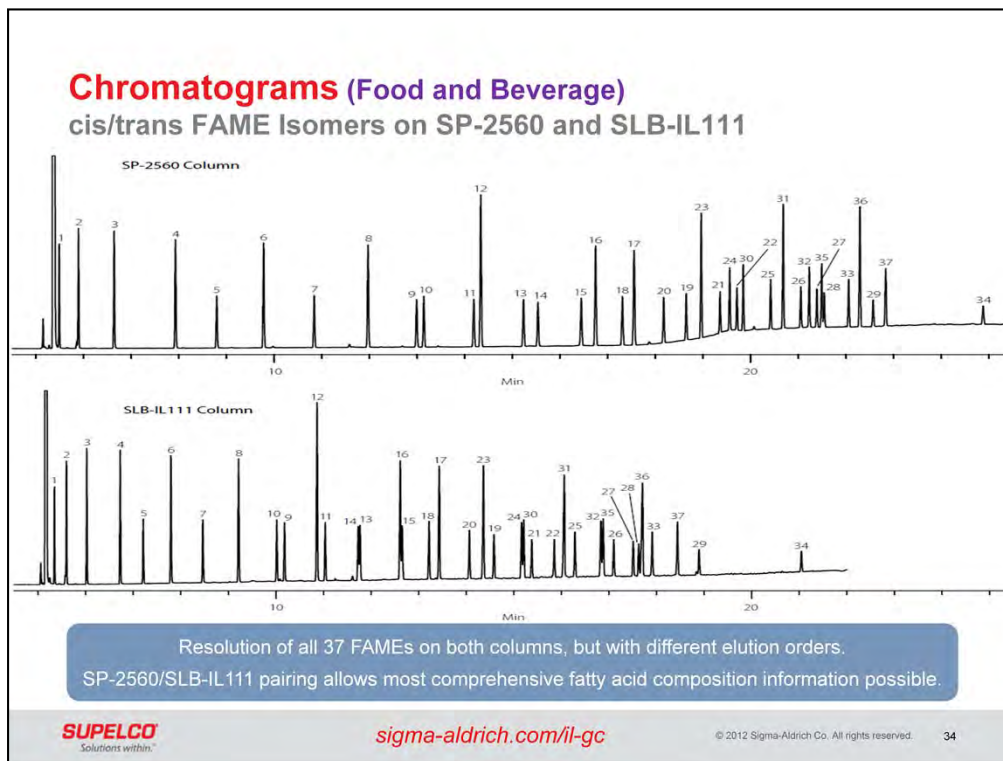
Peak IDs

1. C14:0
2. C16:0
3. C16:1n7
4. C16:2n4
5. C16:3n4
6. C18:0
7. C18:1n9
8. C18:1n7
9. C18:2n6
10. C18:3n4
11. C18:3n3 (ALA)
12. C18:4n3
13. C20:1n9
14. C20:3n3
15. C20:4n3
16. C20:5n3 (EPA)
17. C22:5n3
18. C22:6n3 (DHA)

Conditions

- column: SLB-IL60, 30 m x 0.25 mm I.D., 0.20 μ m (29505-U)
- oven: 170 $^{\circ}$ C, 1 $^{\circ}$ C/min to 225 $^{\circ}$ C
- inj. temp.: 250 $^{\circ}$ C
- detector: FID, 260 $^{\circ}$ C
- carrier gas: helium, 1.2 mL/min
- injection: 1 μ L, 100:1 split
- liner: 4 mm I.D., split/splitless type, wool packed single taper FocusLiner design

[Chromatogram IDs = G005814 (Omegawax, not shown), G006248 (SLB-IL60)]



Trans fat content is reported on nutritional facts panels as part of proper food labeling. It is desirable to use a column which can resolve trans FAME isomers from cis FAME isomers, so trans fat values are not biased high. These chromatograms of C4 to C24 FAMEs on the SP-2560 and SLB-IL111 represent the ultimate in cis/trans FAME analysis. This is because the SP-2560/SLB-IL111 pairing allows the most comprehensive fatty acid composition information possible.

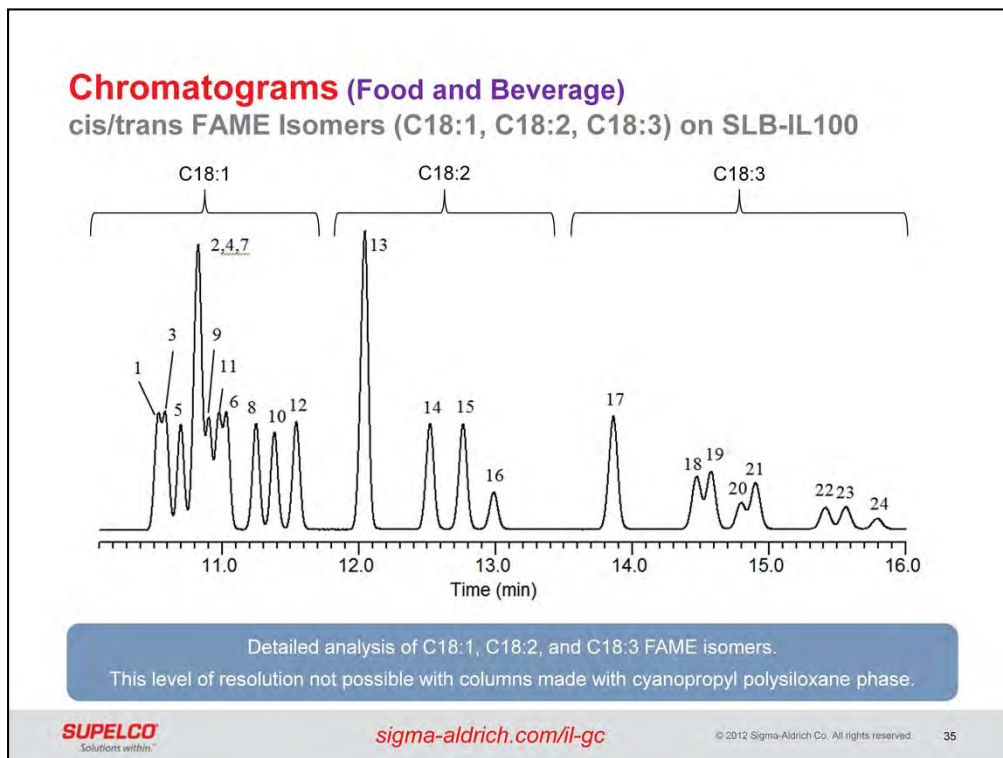
SP-2560 Conditions

- column: SP-2560, 100 m x 0.25 mm I.D., 0.20 μm (24056)
- oven: 140 $^{\circ}\text{C}$ (5 min), 8 $^{\circ}\text{C}/\text{min}$ to 180 $^{\circ}\text{C}$, 4 $^{\circ}\text{C}/\text{min}$ to 210 $^{\circ}\text{C}$, 20 $^{\circ}\text{C}/\text{min}$ to 250 $^{\circ}\text{C}$ (7 min)
- inj. temp.: 250 $^{\circ}\text{C}$
- detector: FID, 250 $^{\circ}\text{C}$
- carrier gas: hydrogen, 40 cm/sec
- injection: 1 μL , 100:1 split
- liner: 4 mm I.D., split type, cup design
- sample: Supelco 37-Component FAME Mix (47885-U)

SLB-IL111 Conditions

- column: SLB-IL111, 100 m x 0.25 mm I.D., 0.20 μm (29647-U)
- oven: 140 $^{\circ}\text{C}$ (5 min), 8 $^{\circ}\text{C}/\text{min}$ to 180 $^{\circ}\text{C}$, 5 $^{\circ}\text{C}/\text{min}$ to 260 $^{\circ}\text{C}$
- detector: FID, 260 $^{\circ}\text{C}$
- All other conditions the same as those used for the SP-2560

[Chromatogram IDs = G005366 (SP-2560), G005367 (SLB-IL111)]



Many regulatory agencies worldwide require content labeling to inform buyers of 'trans fat' levels of foods and some dietary supplements. This is because trans fatty acids have adverse health consequences and no known nutritional benefits over other fats. Some of the most common unsaturated fatty acids are the C18 series. This chromatogram shows a detailed analysis of C18:1, C18:2, and C18:3 fatty acid isomers, as fatty acid methyl esters (FAMES), on a SLB-IL100. This level of resolution is not possible with columns made with cyanopropyl polysiloxane phase.

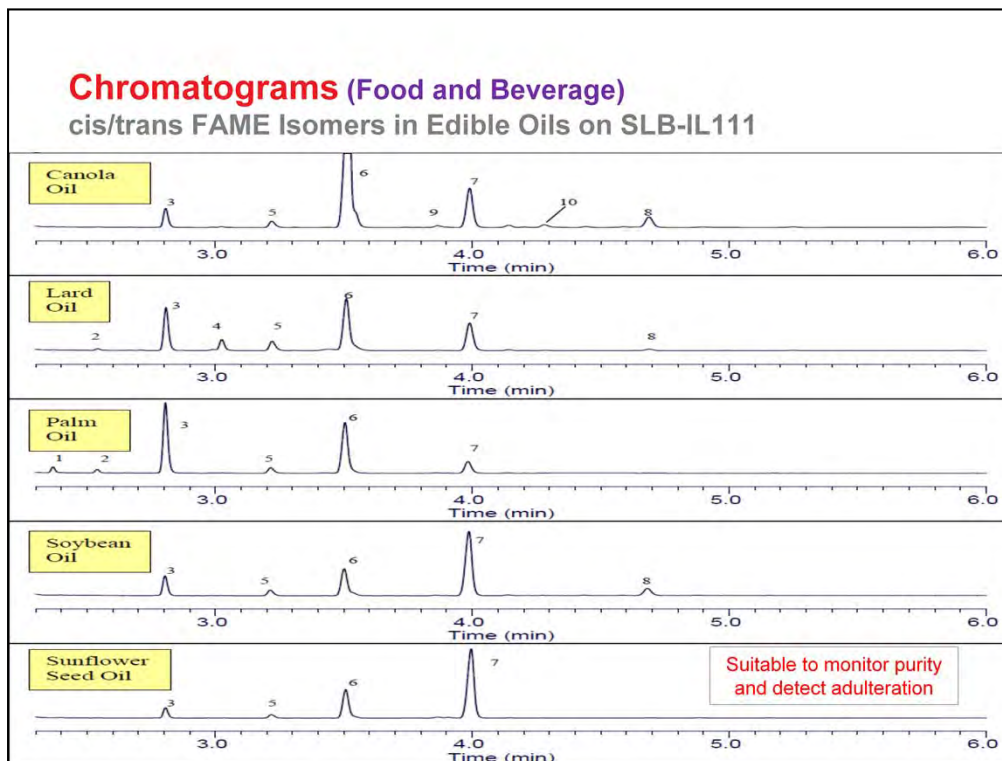
Peak IDs

1. C18:1Δ6t
2. C18:1Δ6c
3. C18:1Δ7t
4. C18:1Δ7c
5. C18:1Δ9t
6. C18:1Δ9c
7. C18:1Δ11t
8. C18:1Δ11c
9. C18:1Δ12t
10. C18:1Δ12c
11. C18:1Δ13t
12. C18:1Δ13c
13. C18:2Δ9t,12t
14. C18:2Δ9c,12t
15. C18:2Δ9t,12c
16. C18:2Δ9c,12c
17. C18:3Δ9t,12t,15t
18. C18:3Δ9t,12t,15c
19. C18:3Δ9t,12c,15t
20. C18:3Δ9c,12c,15t
21. C18:3Δ9c,12t,15t
22. C18:3Δ9c,12t,15c
23. C18:3Δ9t,12c,15c
24. C18:3Δ9c,12c,15c

Conditions

- column: SLB-IL100, 60 m x 0.25 mm I.D., 0.20 μm (28886-U)
- oven: 170 °C
- inj. temp.: 250 °C
- detector: FID, 250 °C
- carrier gas: helium, 30 cm/sec
- injection: 1 μL, 50:1 split
- liner: 4 mm I.D., split type, cup design
- sample: mixture of C18:1, C18:2, and C18:3 FAMES in methylene chloride

[Chromatogram ID = G004386]



Each pure edible oil has a unique combination of FAMEs in specific ratios. Therefore, GC fingerprinting can be used to monitor purity. It can also be used to detect adulteration when a cheaper, inferior oil is added to boost the volume of a premium, higher priced oil. The SLB-IL111 column is able to provide the necessary resolution of key FAME isomers found in several edible oils for effective fingerprinting.

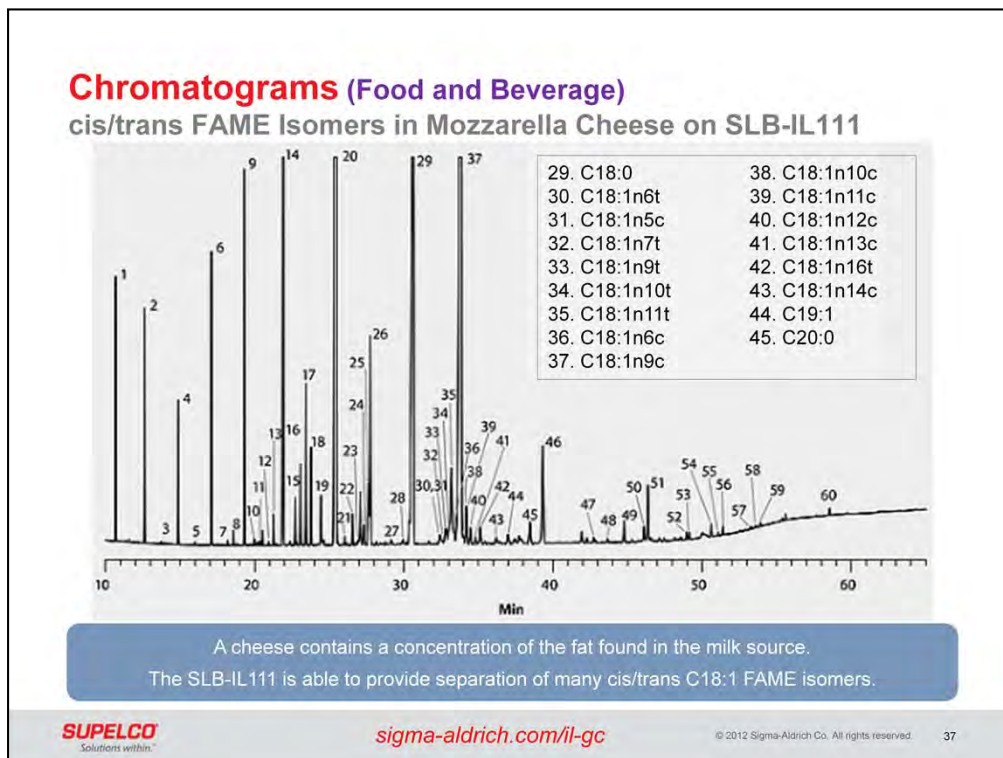
Peak IDs

1. Lauric acid methyl ester (C12:0)
2. Myristic acid methyl ester (C14:0)
3. Palmitic acid methyl ester (C16:0)
4. Palmitoleic acid methyl ester (C16:1)
5. Stearic acid methyl ester (C18:0)
6. Oleic acid methyl ester (C18:1n9c)
7. Linoleic acid methyl ester (C18:2n6c)
8. Linolenic acid methyl ester (C18:3n3)
9. Arachidic acid methyl ester (C20:0)
10. cis-11-Eicosenoic acid methyl ester (C20:1)

Conditions

- column: SLB-IL111, 30 m x 0.25 mm I.D., 0.20 μ m (28927-U)
- oven: 180 $^{\circ}$ C
- inj. temp.: 250 $^{\circ}$ C
- detector: FID, 260 $^{\circ}$ C
- carrier gas: helium, 25 cm/sec
- injection: 1 μ L, 50:1 split
- liner: 4 mm I.D., split type, cup design

[Chromatogram ID = G005480]



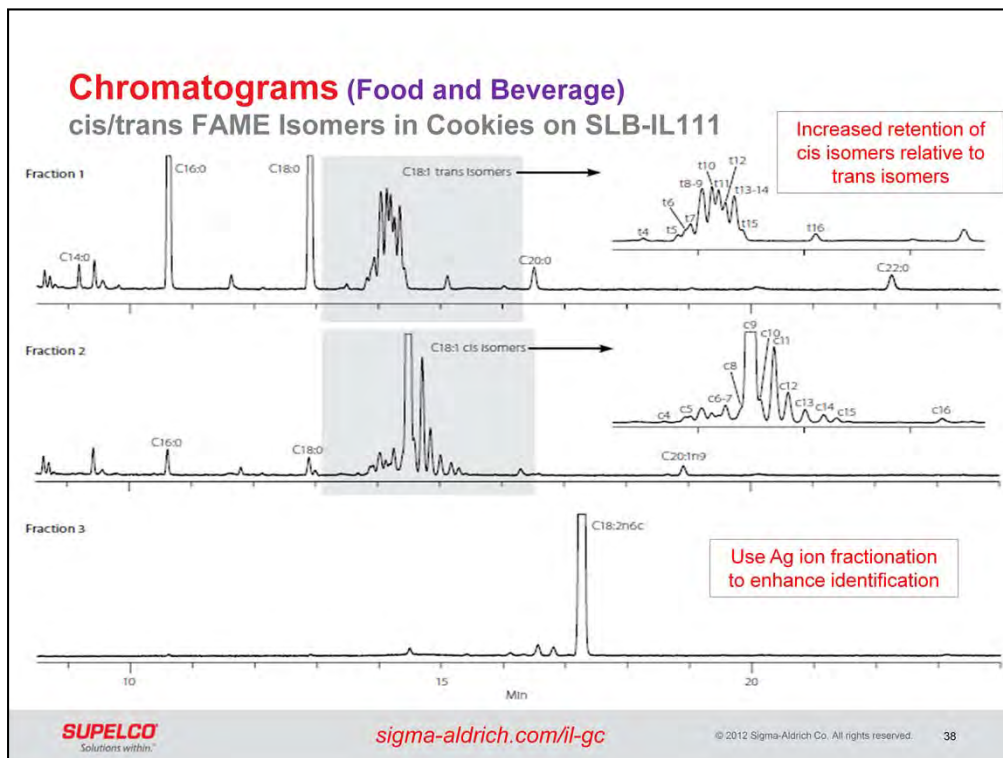
A cheese contains a concentration of the fat found in the milk source. This is because almost all of milk's nutrients are retained during the process of manufacturing cheese. This chromatogram shows the analysis of fatty acids (as fatty acid methyl esters) extracted from a mozzarella cheese made with buffalo milk. The SLB-IL111 is able to provide separation of many cis/trans C18:1 FAME isomers.

Chromatogram courtesy of Prof. Luigi Mondello (Univ. of Messina, Italy)

Conditions

- column: SLB-IL111, 100 m x 0.25 mm I.D., 0.20 μm (29647-U)
- oven: 70 $^{\circ}\text{C}$ (4 min), 12 $^{\circ}\text{C}/\text{min}$ to 160 $^{\circ}\text{C}$ (25 min), 4 $^{\circ}\text{C}/\text{min}$ to 220 $^{\circ}\text{C}$
- inj. temp.: 230 $^{\circ}\text{C}$
- detector: FID, 240 $^{\circ}\text{C}$
- carrier gas: hydrogen, 40 cm/sec
- injection: 0.2 μL , 10:1 split
- sample: FAMES from 100 mg mozzarella (made with buffalo milk) transesterified in sodium methoxide/methanol + boron trifluoride

[Chromatogram ID = G006060]

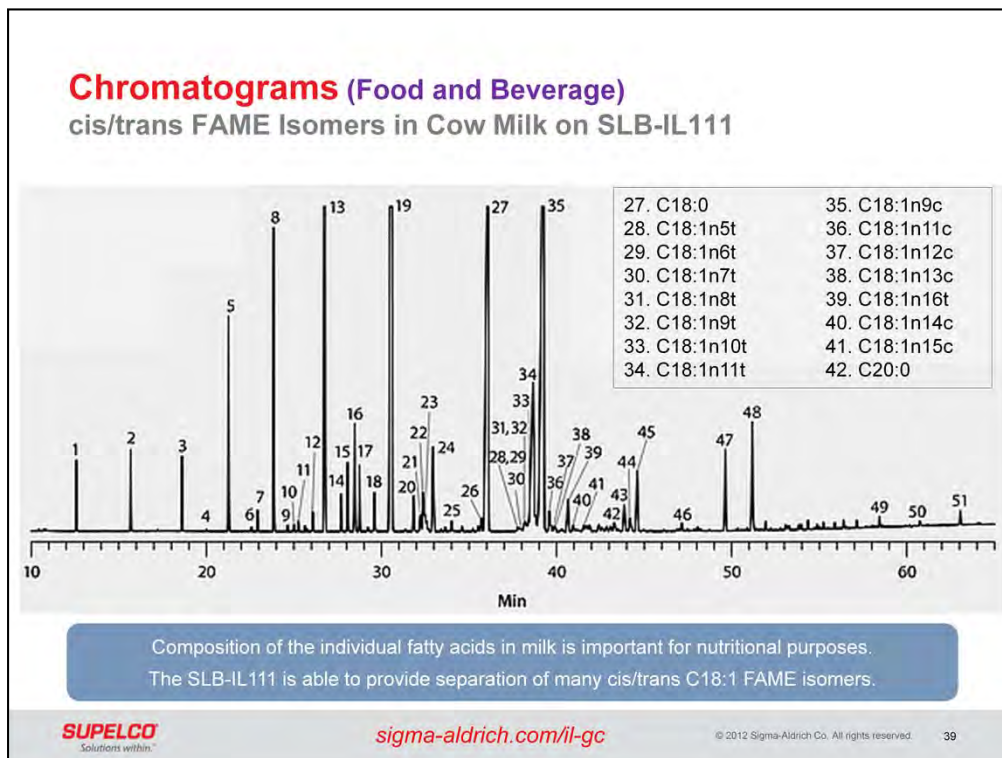


A sample of commercially purchased cookies was ground, and fatty acids were extracted, methylated, fractionated, and analyzed with GC-FID using the SLB-IL111. The nutritional label for the cookies included partially hydrogenated cottonseed and soybean oils as ingredients. Based on this information, the fatty acid profile obtained for this sample was as expected; with cottonseed oil accounting for the small amount of C14:0 FAME, and the soybean oil as the source of the small amount of C22:0 FAME detected. Both oils contributed to the higher levels of the C16:0, C18:0 and C18:1 FAMEs. Note the presence of the C18:1 trans isomers in fraction 1. These are the result of the partial hydrogenation of these oils.

Conditions

- sample/matrix: 1 g of commercially purchased cookies was ground and subjected to acid digestion and alkali hydrolysis, followed by methylation as described in AOCS Official Method Ce 1k-09
- SPE tube: Discovery Ag-Ion SPE tubes, 750 mg/6 mL (54225-U)
- conditioning: 4 mL of acetone; allow solvent to gravity drip completely through tube; discard eluant; 4 mL of hexane; allow solvent to gravity drip completely through tube; discard eluant
- sample addition: 1 mL of extract; discard any eluant that drips through tube elution: (Fraction 1) 6 mL of hexane:acetone (96:4); collect eluant in a fresh container with slight vacuum; (Fraction 2) 4 mL of hexane: acetone (90:10); collect eluant in a fresh container with slight vacuum; (Fraction 3) 4 mL of 100% acetone; collect eluant in a fresh container with slight vacuum
- eluate: post-treatment: evaporate each fraction at room temperature using nitrogen; reconstitute each fraction to 1 mL of hexane
- column: SLB-IL111, 100 m x 0.25 mm I.D., 0.20 μ m (29647-U)
- oven: 168 $^{\circ}$ C
- inj. temp.: 250 $^{\circ}$ C
- detector: FID, 250 $^{\circ}$ C
- carrier gas: hydrogen, 1 mL/min
- injection: 1 μ L, 10:1 split
- liner: 4 mm I.D., split type, single taper wool packed FocusLiner design

[Chromatogram ID = G005622]



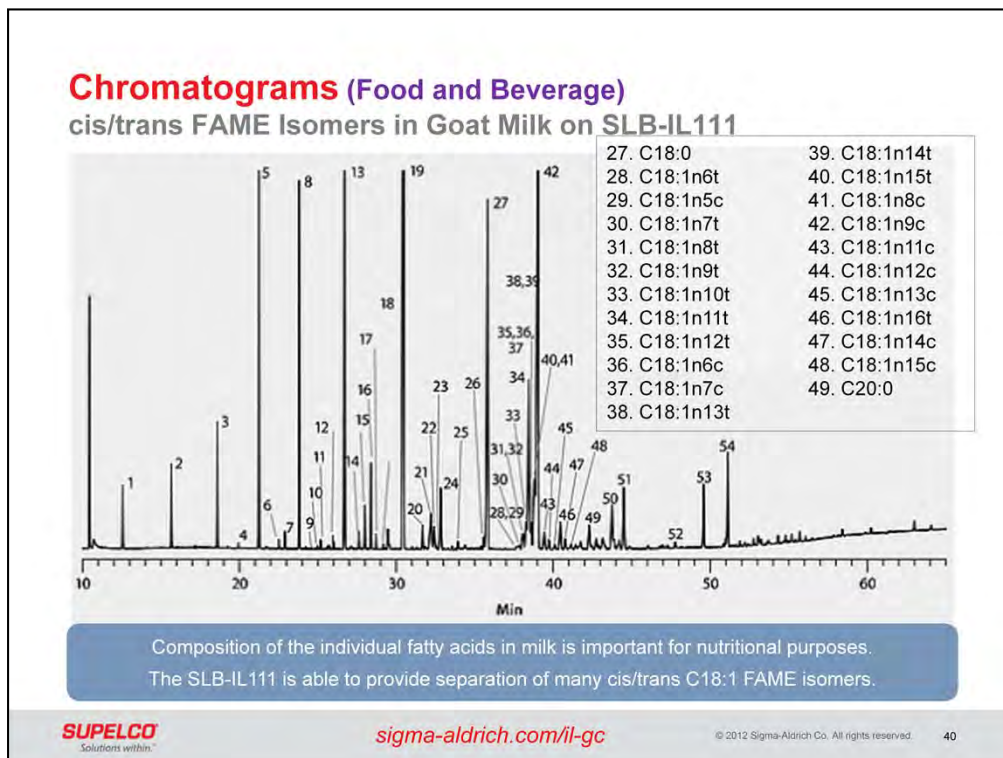
Milk contains a wide variety of fats, predominantly in the form of triglycerides. The composition of the individual fatty acids is important for nutritional purposes. To obtain this information, the triglycerides are broken into the component fatty acids and glycerol, then the fatty acids converted to fatty acid methyl esters (FAMES) prior to GC analysis. This chromatogram shows the analysis of fatty acids (as fatty acid methyl esters) extracted from cow milk. The SLB-IL111 is able to provide separation of many cis/trans C18:1 FAME isomers.

Chromatogram courtesy of Prof. Luigi Mondello (Univ. of Messina, Italy)

Conditions

- column: SLB-IL111, 100 m x 0.25 mm I.D., 0.20 μm (29647-U)
- oven: 50 $^{\circ}\text{C}$ (4 min), 8 $^{\circ}\text{C}/\text{min}$ to 160 $^{\circ}\text{C}$ (25 min), 4 $^{\circ}\text{C}/\text{min}$ to 220 $^{\circ}\text{C}$
- inj. temp.: 230 $^{\circ}\text{C}$
- detector: FID, 240 $^{\circ}\text{C}$
- carrier gas: hydrogen, 40 cm/sec
- injection: 0.2 μL , 10:1 split
- sample: FAMES from 100 mg cow milk transesterified in sodium methoxide/methanol + boron trifluoride

[Chromatogram ID = G006061]



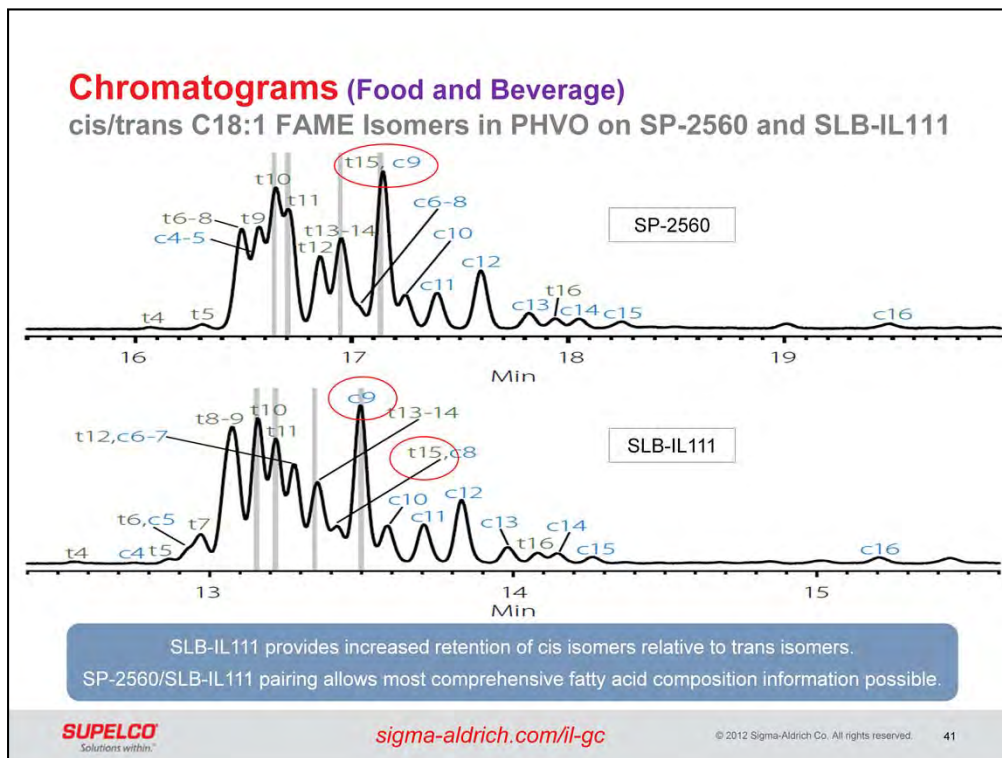
Milk contains a wide variety of fats, predominantly in the form of triglycerides. The composition of the individual fatty acids is important for nutritional purposes. To obtain this information, the triglycerides are broken into the component fatty acids and glycerol, then the fatty acids converted to fatty acid methyl esters (FAMES) prior to GC analysis. This chromatogram shows the analysis of fatty acids (as fatty acid methyl esters) extracted from goat milk. The SLB-IL111 is able to provide separation of many cis/trans C18:1 FAME isomers.

Chromatogram courtesy of Prof. Luigi Mondello (Univ. of Messina, Italy)

Conditions

- column: SLB-IL111, 100 m x 0.25 mm I.D., 0.20 μ m (29647-U)
- oven: 50 °C (4 min), 8 °C/min to 160 °C (25 min), 4 °C/min to 220 °C
- inj. temp.: 230 °C
- detector: FID, 240 °C
- carrier gas: hydrogen, 40 cm/sec
- injection: 0.2 μ L, 10:1 split
- sample: FAMES from 100 mg goat milk transesterified in sodium methoxide/methanol + boron trifluoride

[Chromatogram ID = G006062]



Columns made with cyanopropyl polysiloxane phases are traditionally used for the separation of cis and trans geometric positional isomers of fatty acids methyl esters (FAMES). The 100 m SP-2560 column is a workhorse for this application. This slide shows chromatograms of a partially hydrogenated vegetable oil (PHVO) sample run on the 100 m SP-2560 and the 100 m SLB-IL111. When comparing FAME isomers with the same degree of unsaturation, the SLB-IL111 provides increased retention of cis isomers relative to trans isomers with the double bond at the same location. The SLB-IL111 was able to provide resolution of C18:1n9c from C18:1n15t, a separation not possible with the SP-2560. The SLB-IL111 offered improved resolution of some isomers that cannot be completely resolved with the SP-2560 either.

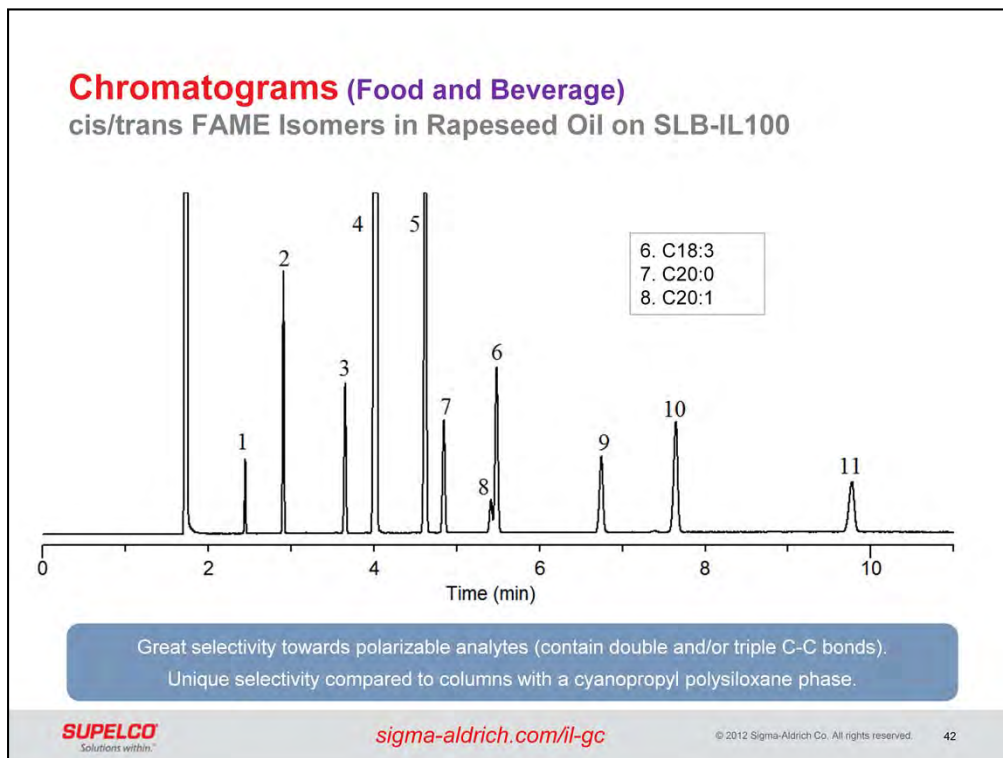
SP-2560 Conditions

- column: SP-2560, 100 m x 0.25 mm I.D., 0.20 μm (24056)
- oven: 180 $^{\circ}\text{C}$ isothermal
- inj. temp: 250 $^{\circ}\text{C}$
- detector: FID, 250 $^{\circ}\text{C}$
- carrier gas: hydrogen, 1 mL/min
- injection: 1 μL , 100:1 split
- liner: 4 mm I.D., split liner with cup (2051001)

SLB-IL111 Conditions

- column: SLB-IL111, 100 m x 0.25 mm I.D., 0.20 μm (29647-U)
- oven: 168 $^{\circ}\text{C}$ isothermal
- All other conditions the same as those used for the SP-2560

[Chromatogram IDs = G005287 (SP-2560), G005290 (SLB-IL111)]



Rapeseed oil is a simple vegetable oil that contains a series of saturated and unsaturated fatty acids ranging from C14 through C24 in carbon number. Monitoring the elution locations of C18:3 (peak 6), C20:0 (peak 7), and C20:1 (peak 8) relative to each other, as well as the other FAMEs, is an indication of a column's relative strength of dipole-induced dipole interactions. The SLB-IL100 column has great selectivity towards polarizable analytes (contain double and/or triple C-C bonds). It provides a unique selectivity compared to columns with a cyanopropyl polysiloxane phase.

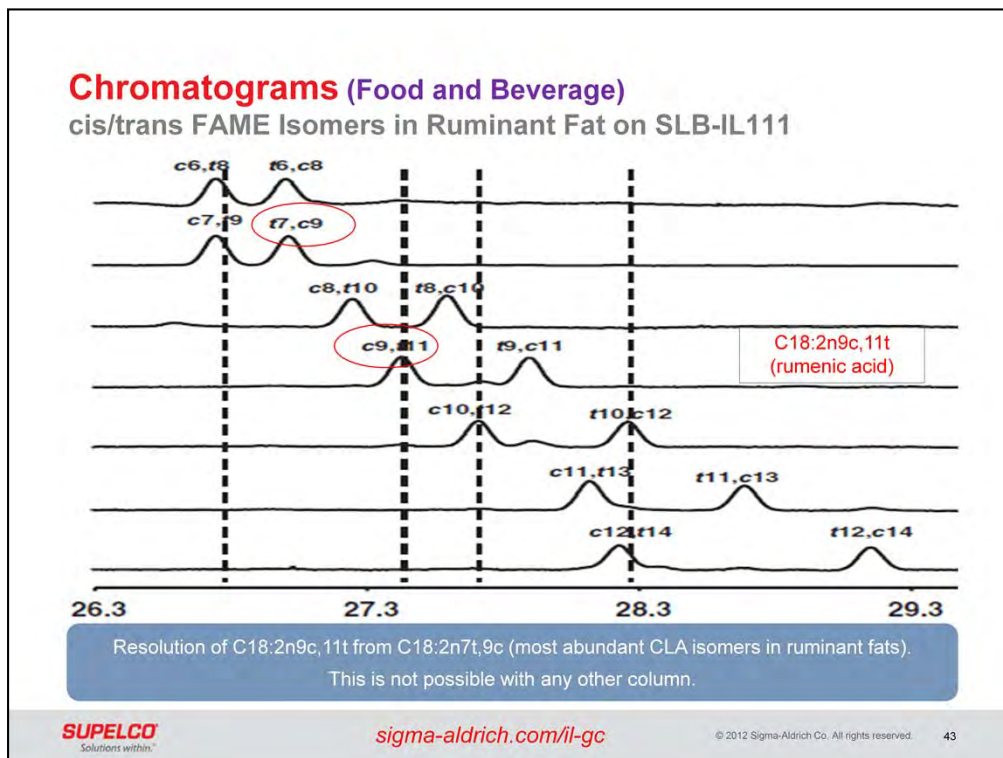
Peak IDs

1. Myristic (C14:0)
2. Palmitic (C16:0)
3. Stearic (C18:0)
4. Oleic (C18:1n9c)
5. Linoleic (C18:2)
6. Linolenic (C18:3)
7. Arachidic (C20:0)
8. cis-11-Eicosenoic (C20:1)
9. Behenic (C22:0)
10. Erucic (C22:1)
11. Lignoceric (C24:0)

Conditions

- column: SLB-IL100, 30 m x 0.25 mm I.D., 0.20 μ m (28884-U)
- oven: 180 $^{\circ}$ C
- inj. temp.: 250 $^{\circ}$ C
- detector: FID, 250 $^{\circ}$ C
- carrier gas: helium, 30 cm/sec @ 180 $^{\circ}$ C
- injection: 1 μ L, 100:1 split
- liner: 4 mm I.D., split type, cup design
- sample: Rapeseed oil FAME mix, 5 mg/mL total FAMEs in methylene chloride

[Chromatogram ID = G004218]



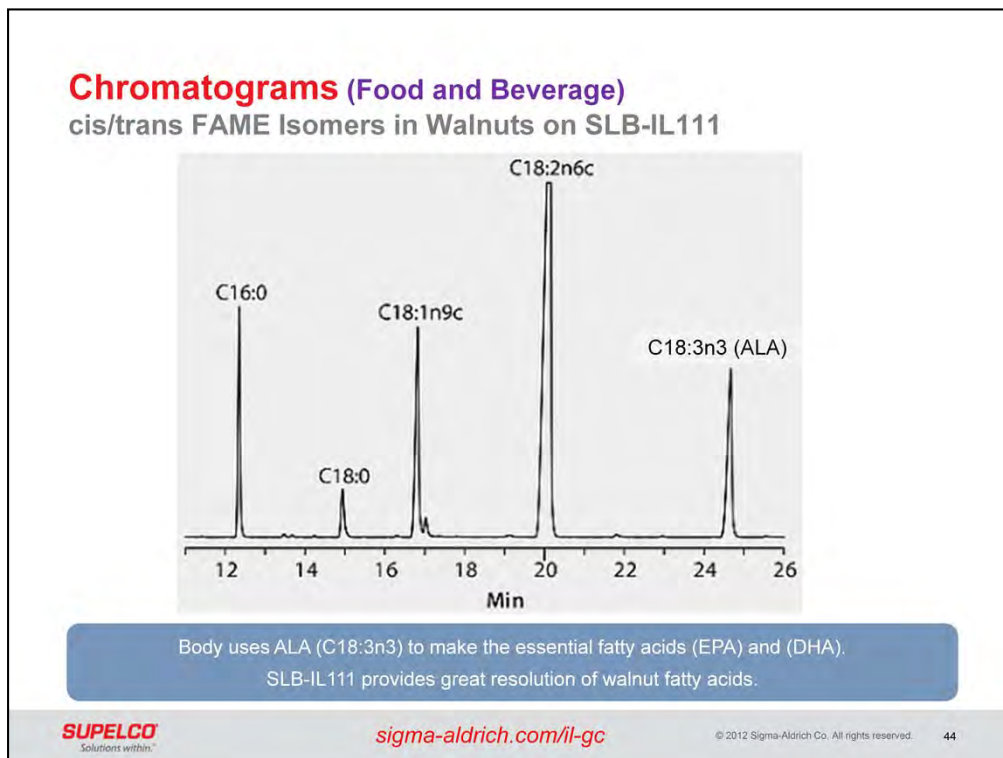
The stomachs of several mammal species have four compartments. These mammals are known as ruminants, and include cows, sheep, goats, and deer. Conjugated linoleic acid (CLA) isomers are C18:2 fatty acids in which a single C-C bond separates the two double bonds. C18:2n7t,9c and C18:2n9c,11t are the two most abundant CLA isomers found in ruminant fats. The C18:2n9c,11t isomer is called rumenic acid, and may have anti-carcinogenic properties. The SLB-IL111 is able to separate these two CLA isomers, a feat that cannot be accomplished on any other column. This allows the more accurate reporting of rumenic acid concentration as it is not biased high from the co-elution of the C18:2n7t,9c isomer.

Conditions

- column: SLB-IL111, 100 m x 0.25 mm I.D., 0.20 μ m (29647-U)
- oven: 168 °C
- carrier gas: hydrogen, 26 cm/sec

Data reported and shown in P. Delmonte, A-R.F. Kia, J.K.G. Kramer, M.M. Mossoba, L. Sidisky, and J.I. Rader, "Separation Characteristics of Fatty Acid Methyl Esters Using SLBIL111, A New Ionic Liquid Coated Capillary Gas Chromatographic Column" *J. Chromatogr. A* 1218 (2011) p. 545.

[Chromatogram ID = n/a]



Nuts are considered nutrient dense foods and their consumption has been associated with a reduced risk of coronary heart disease. The health benefits of nuts are partially attributable to their high content of unsaturated fatty acids. For example, alpha-linolenic acid (ALA), an unsaturated fatty acid found in flaxseeds and walnuts, is a precursor to the formation within the body of the essential fatty acids eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA). This application illustrates the GC analysis of fatty acids extracted from walnuts, considered a significant plant source of (ALA). The SLB-IL111 provides great resolution.

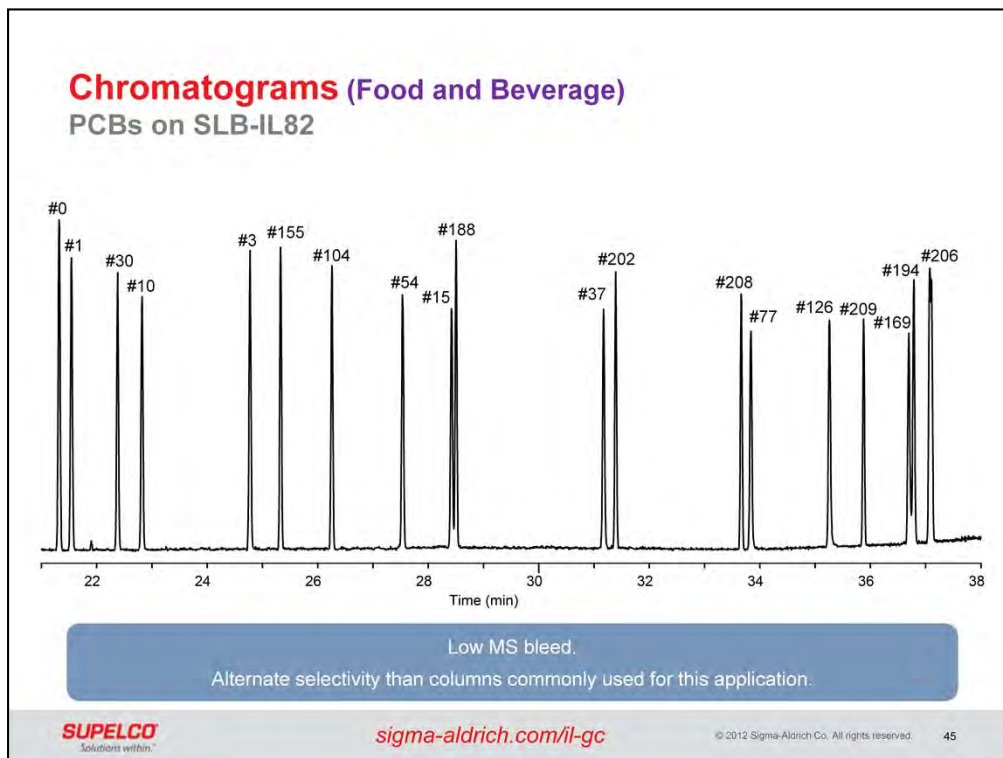
Peak IDs

1. Palmitic acid methyl ester (C16:0)
2. Stearic acid methyl ester (C18:0)
3. Oleic acid methyl ester (C18:1n9c)
4. Linoleic acid methyl ester (C18:2n6c) [LA]
5. alpha-Linolenic acid methyl ester (C18:3n3) [ALA]

Conditions

- column: SLB-IL111, 100 m x 0.25 mm I.D., 0.20 μ m (29647-U)
- oven: 168 $^{\circ}$ C isothermal
- inj. temp.: 250 $^{\circ}$ C
- detector: FID, 260 $^{\circ}$ C
- carrier gas: helium, 1.0 mL/min
- injection: 1 μ L, 100:1 split
- liner: 4 mm I.D., split/splitless type, wool packed single taper FocusLiner design
- sample: extract of walnuts

[Chromatogram ID = G005823]



Polychlorinated biphenyls (PCBs), classified as persistent organic pollutants (POPs), have been found in several food types, such as milk. This chromatogram of 19 PCBs was analyzed on the SLB-IL82. In addition to the low level of MS bleed, the SLB-IL82 offers alternate selectivity than the columns commonly used for this application.

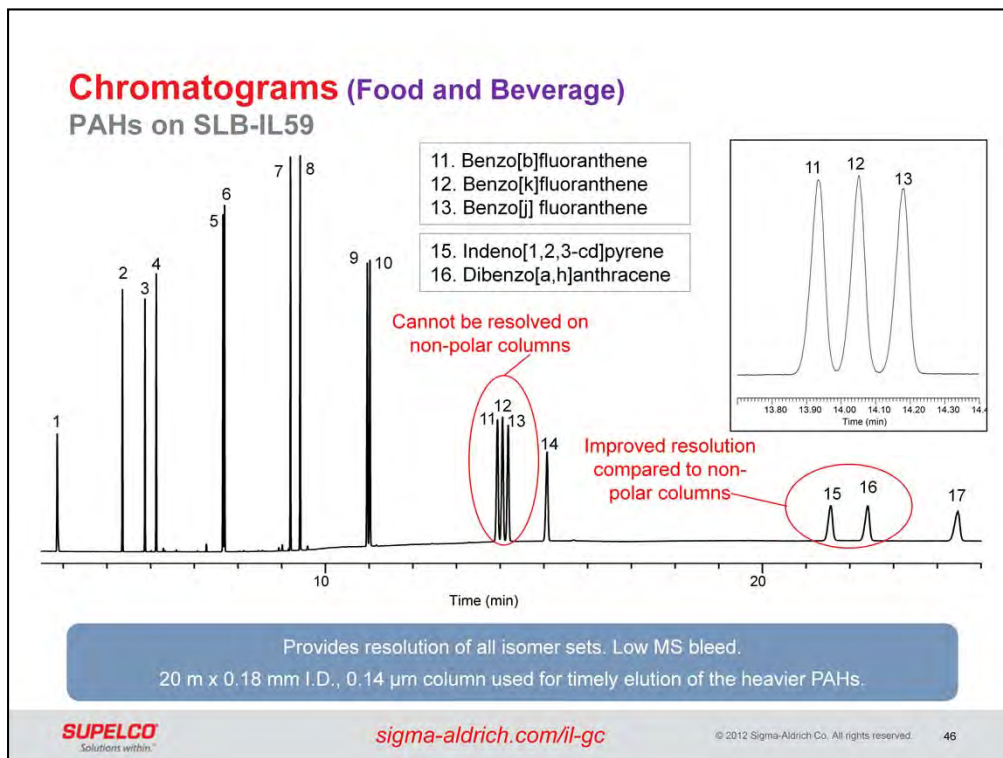
Peak IDs

- #0 = Biphenyl
- #1 = 2-monochlorobiphenyl
- #3 = 4-monochlorobiphenyl
- #10 = 2,6-dichlorobiphenyl
- #15 = 4,4'-dichlorobiphenyl
- #30 = 2,4,6-trichlorobiphenyl
- #37 = 3,4,4'-trichlorobiphenyl
- #54 = 2,2',6,6'-tetrachlorobiphenyl
- #77 = 3,3',4,4'-tetrachlorobiphenyl
- #104 = 2,2',4,6,6'-pentachlorobiphenyl
- #126 = 3,3',4,4',5-pentachlorobiphenyl
- #155 = 2,2',4,4',6,6'-hexachlorobiphenyl
- #169 = 3,3',4,4',5,5'-hexachlorobiphenyl
- #188 = 2,2',3,4',5,6,6'-heptachlorobiphenyl
- #194 = 2,2',3,3',4,4',5,5'-octachlorobiphenyl
- #202 = 2,2',3,3',5,5',6,6'-octachlorobiphenyl
- #206 = 2,2',3,3',4,4',5,5',6-nonachlorobiphenyl
- #208 = 2,2',3,3',4,5,5',6,6'-nonachlorobiphenyl
- #209 = Decachlorobiphenyl

Conditions

- column: SLB-IL82, 30 m x 0.25 mm I.D., 0.20 μ m (29479-U)
- oven: 50 $^{\circ}$ C (2 min), 5 $^{\circ}$ C/min to 260 $^{\circ}$ C
- inj. temp.: 250 $^{\circ}$ C
- detector: MSD, m/z = 100-550
- carrier gas: helium, 1.0 mL/min
- injection: 1 μ L, splitless (splitter open at 1 min)
- liner: 4 mm I.D., split/splitless type, single taper design
- sample: PCB congener mix, each analyte at 2.5 ppm in n-hexane

[Chromatogram ID = G006237]



Polycyclic aromatic hydrocarbons (PAHs) are produced as by-products of cooking meat at high temperatures. Several PAHs are identified as carcinogens. The PAHs of interest include several isomer sets. This chromatogram of 19 PAHs on the SLB-IL59 highlights the ability of this column to provide resolution of all isomer sets, and exhibit low MS bleed. A 20 m x 0.18 mm I.D., 0.14 μ m column was used for the timely elution of the heavier PAHs.

Peak IDs

1. Naphthalene
2. Acenaphthene
3. Acenaphthylene
4. Fluorene
5. Phenanthrene
6. Anthracene
7. Fluoranthene
8. Pyrene
9. Benzo[a]anthracene
10. Chrysene
11. Benzo[b]fluoranthene
12. Benzo[k]fluoranthene
13. Benzo[j] fluoranthene
14. Benzo[a]pyrene
15. Indeno[1,2,3-cd]pyrene
16. Dibenzo[a,h]anthracene
17. Benzo[g,h,i]perylene

Conditions

- column: SLB-IL59, 20 m x 0.18 mm I.D., 0.14 μ m (custom)
- oven: 65 °C (0.5 min), 25 °C/min to 300 °C (20 min)
- inj. temp.: 265 °C
- carrier gas: helium, 50 psi constant pressure
- detector: MSD, interface at 300 °C, m/z = 50-500
- injection: 1 μ L, splitless (1 min)
- liner: 4 mm I.D., split/splitless type, wool packed single taper FocusLiner design
- sample: each PAH at 10 μ g/mL in methylene chloride

[Chromatogram ID = G006238]

Agenda

- Chromatograms
- Summary / Related Products / Resources

- Environmental
- Petroleum
- Biofuel
- Chemical
- Agriculture
- Food and Beverage
- **Flavor and Fragrance**
- Clinical
- General Analytical

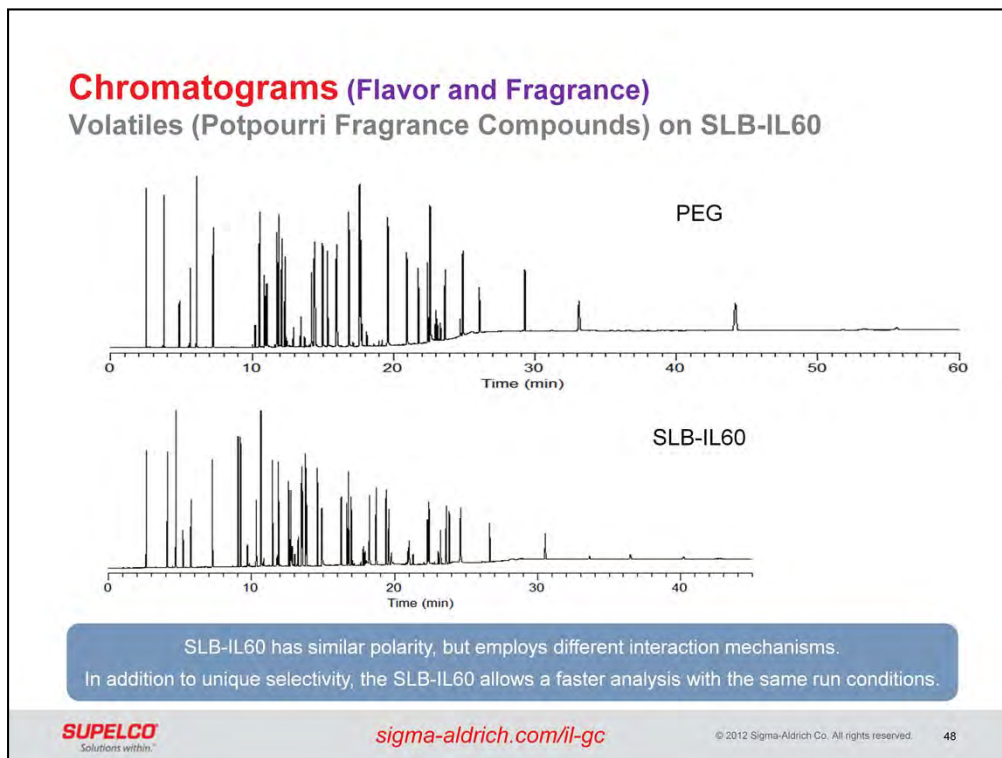
Analyte IDs and GC conditions are included in the speaker notes for most chromatograms. Otherwise, enter chromatogram ID from speaker notes into the search bar at <sigma-aldrich.com>.

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Chromatograms – Flavor and Fragrance Applications



Columns made with polyethylene glycol (PEG) phases are commonly used for fragrance compounds. This slide shows the analysis of a mixture of fragrance compounds on a PEG and also on a SLB-IL60. The SLB-IL60 has similar polarity, but employs different interaction mechanisms. In addition to unique selectivity, the SLB-IL60 allows a faster analysis with the same run conditions.

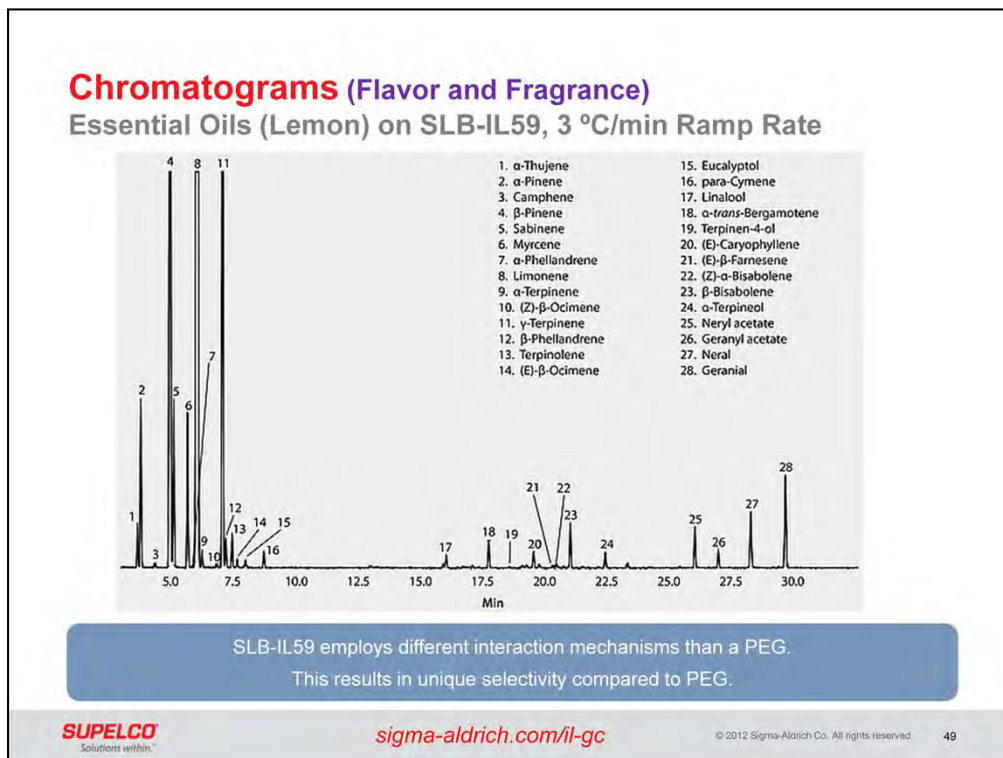
SUPELCOWAX 10 Conditions

- column: SUPELCOWAX 10, 30 m x 0.25 mm I.D., 0.25 μ m (24079)
- oven: 50 $^{\circ}$ C, 8 $^{\circ}$ C/min to 270 $^{\circ}$ C (35 min)
- inj. temp.: 250 $^{\circ}$ C
- detector: FID, 280 $^{\circ}$ C
- carrier gas: helium, 25 cm/sec set at 110 $^{\circ}$ C
- injection: 0.1 μ L, 100:1 split
- liner: 4 mm I.D., split type, cup design
- sample: mixture of potpourri fragrance compounds, neat

SLB-IL60 Conditions

- column: SLB-IL60, 30 m x 0.25 mm I.D., 0.20 μ m (29505-U)
- oven: 50 $^{\circ}$ C, 8 $^{\circ}$ C/min to 270 $^{\circ}$ C (20 min)
- All other conditions the same as those used for the SUPELCOWAX 10

[Chromatogram IDs = G006084 (SUPELCOWAX 10), G006080 (SLB-IL60)]



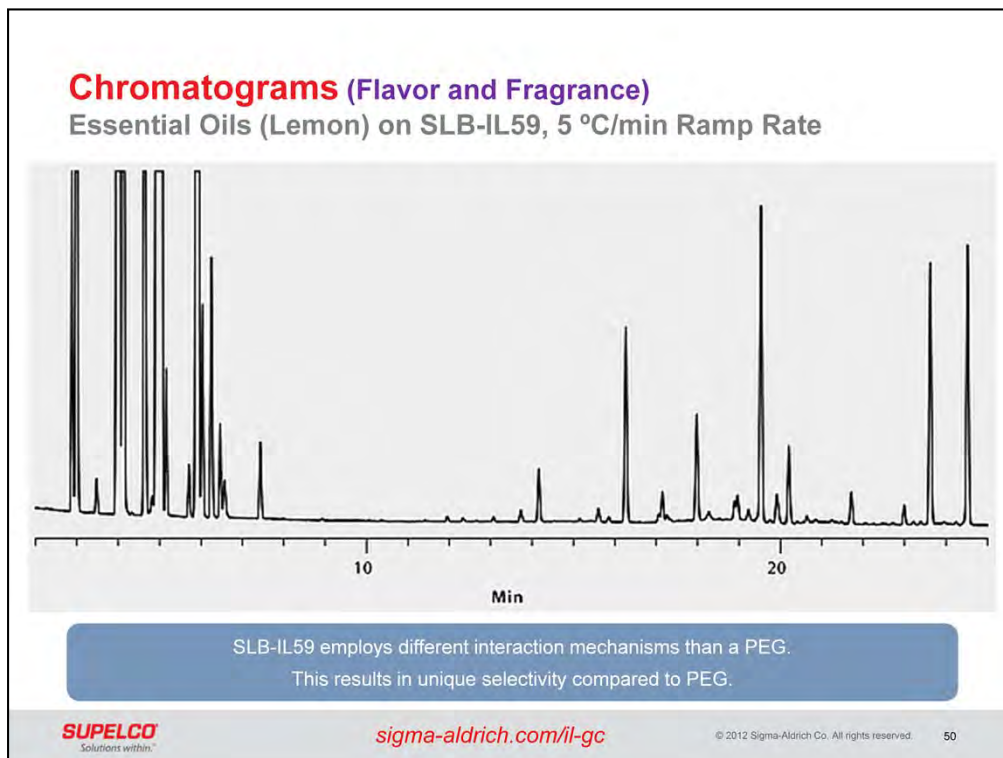
Essential oils are complex mixtures of many compounds. They have different olfactory properties that make some more valuable than others. Smell and taste alone may not be adequate to identify one type from another. GC is a useful tool for performing fingerprinting analysis to identify the type. Columns made with polyethylene glycol (PEG) phases are commonly used. This slide shows the analysis of a lemon essential oil on a SLB-IL59, which employs different interaction mechanisms than a PEG. This results in unique selectivity compared to PEG.

Chromatogram courtesy of Prof. Luigi Mondello (Univ. of Messina, Italy)

Conditions

- column: SLB-IL59, 30 m x 0.25 mm I.D., 0.20 μ m (28891-U)
- oven: 50 °C, 3 °C/min to 300 °C
- detector: FID
- carrier gas: helium, 30 cm/sec
- sample: lemon essential oil

[Chromatogram ID = G005897]



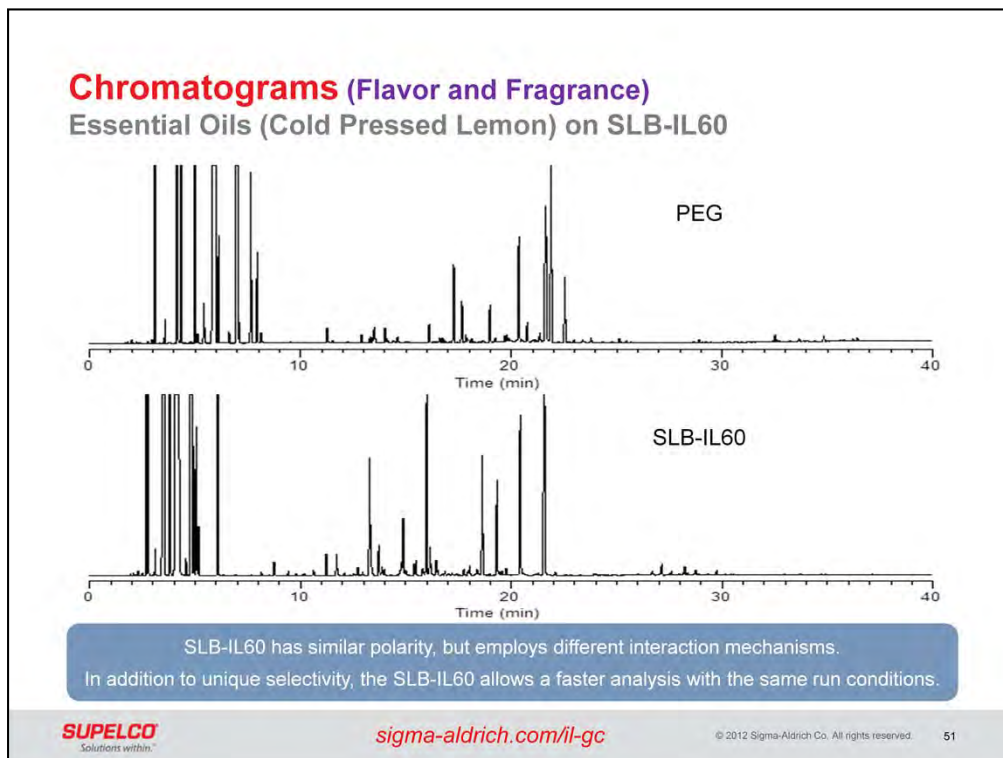
Essential oils are complex mixtures of many compounds. They have different olfactory properties that make some more valuable than others. Smell and taste alone may not be adequate to identify one type from another. GC is a useful tool for performing fingerprinting analysis to identify the type. Columns made with polyethylene glycol (PEG) phases are commonly used. This slide shows the analysis of a lemon essential oil on a SLB-IL59, which employs different interaction mechanisms than a PEG. This results in unique selectivity compared to PEG.

Chromatogram courtesy of Prof. Luigi Mondello (Univ. of Messina, Italy)

Conditions

- column: SLB-IL59, 30 m x 0.25 mm I.D., 0.20 µm (28891-U)
- oven: 50 °C, 5 °C/min to 300 °C
- inj. temp.: 250 °C
- detector: FID, 305 ° C
- carrier gas: helium, 40 cm/sec
- injection: 1 µL, 100:1 split
- sample: lemon essential oil, diluted 1:10 in hexane

[Chromatogram ID = G006065]



Essential oils are complex mixtures of many compounds. They have different olfactory properties that make some more valuable than others. Smell and taste alone may not be adequate to identify one type from another. GC is a useful tool for performing fingerprinting analysis to identify the type. Columns made with polyethylene glycol (PEG) phases are commonly used. This slide shows the analysis of a cold pressed lemon essential oil on a PEG and also on a SLB-IL60. The SLB-IL60 has similar polarity, but employs different interaction mechanisms. In addition to unique selectivity, the SLB-IL60 allows a faster analysis with the same run conditions.

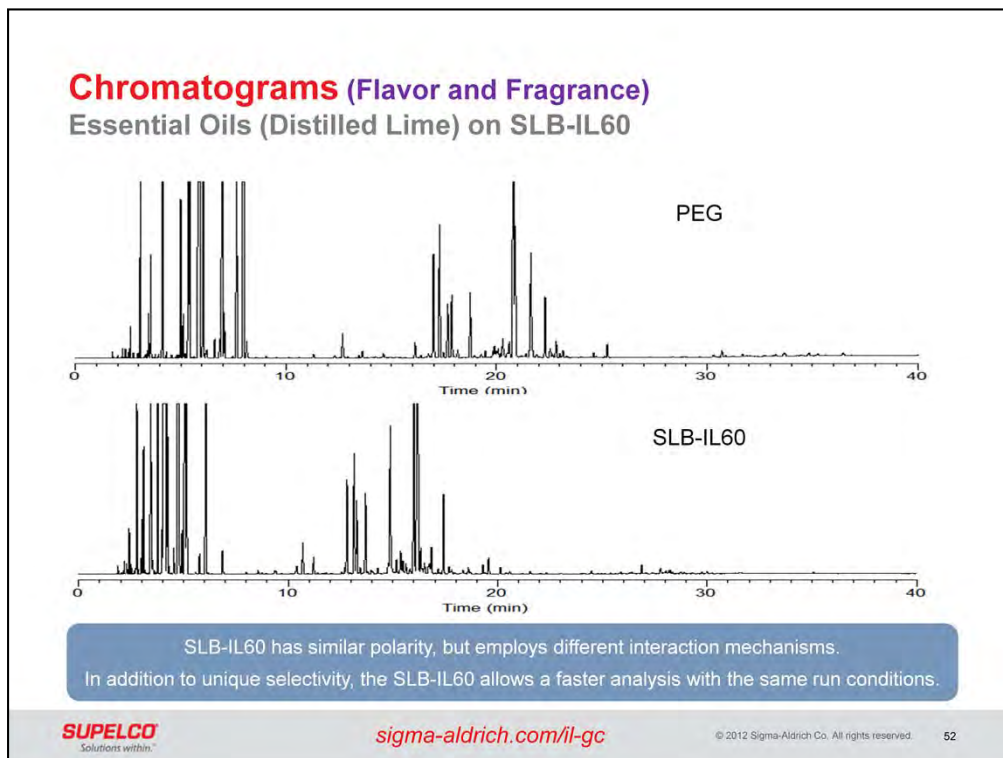
SUPELCO WAX 10 Conditions

- column: SUPELCO WAX 10, 30 m x 0.25 mm I.D., 0.25 μ m (24079)
- oven: 75 $^{\circ}$ C (4 min), 4 $^{\circ}$ C/min to 200 $^{\circ}$ C (10 min)
- inj. temp.: 250 $^{\circ}$ C
- detector: FID, 250 $^{\circ}$ C
- carrier gas: helium, 25 cm/sec set at 110 $^{\circ}$ C
- injection: 0.1 μ L, 100:1 split
- liner: 4 mm I.D., split type, cup design
- sample: cold pressed lemon essential oil, neat

SLB-IL60 Conditions

- column: SLB-IL60, 30 m x 0.25 mm I.D., 0.20 μ m (29505-U)
- All other conditions the same as those used for the SUPELCO WAX 10

[Chromatogram IDs = G006081 (SUPELCO WAX 10), G006078 (SLB-IL60)]



Essential oils are complex mixtures of many compounds. They have different olfactory properties that make some more valuable than others. Smell and taste alone may not be adequate to identify one type from another. GC is a useful tool for performing fingerprinting analysis to identify the type. Columns made with polyethylene glycol (PEG) phases are commonly used. This slide shows the analysis of a distilled lime essential oil on a PEG and also on a SLB-IL60. The SLB-IL60 has similar polarity, but employs different interaction mechanisms. In addition to unique selectivity, the SLB-IL60 allows a faster analysis with the same run conditions.

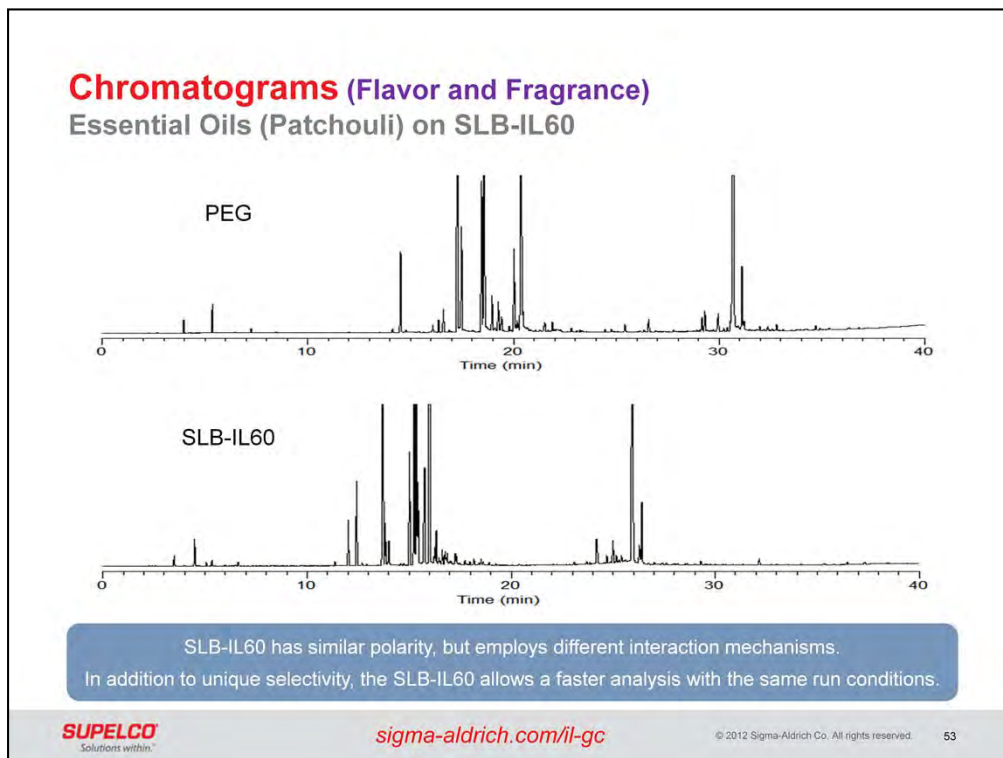
SUPELCO WAX 10 Conditions

- column: SUPELCO WAX 10, 30 m x 0.25 mm I.D., 0.25 μ m (24079)
- oven: 75 $^{\circ}$ C (4 min), 4 $^{\circ}$ C/min to 200 $^{\circ}$ C (10 min)
- inj. temp.: 250 $^{\circ}$ C
- detector: FID, 250 $^{\circ}$ C
- carrier gas: helium, 25 cm/sec set at 110 $^{\circ}$ C
- injection: 0.1 μ L, 100:1 split
- liner: 4 mm I.D., split type, cup design
- sample: distilled lime essential oil, neat

SLB-IL60 Conditions

- column: SLB-IL60, 30 m x 0.25 mm I.D., 0.20 μ m (29505-U)
- All other conditions the same as those used for the SUPELCO WAX 10

[Chromatogram IDs = G006082 (SUPELCO WAX 10), G006079 (SLB-IL60)]



Essential oils are complex mixtures of many compounds. They have different olfactory properties that make some more valuable than others. Smell and taste alone may not be adequate to identify one type from another. GC is a useful tool for performing fingerprinting analysis to identify the type. Columns made with polyethylene glycol (PEG) phases are commonly used. This slide shows the analysis of a patchouli essential oil on a PEG and also on a SLB-IL60. The SLB-IL60 has similar polarity, but employs different interaction mechanisms. In addition to unique selectivity, the SLB-IL60 allows a faster analysis with the same run conditions.

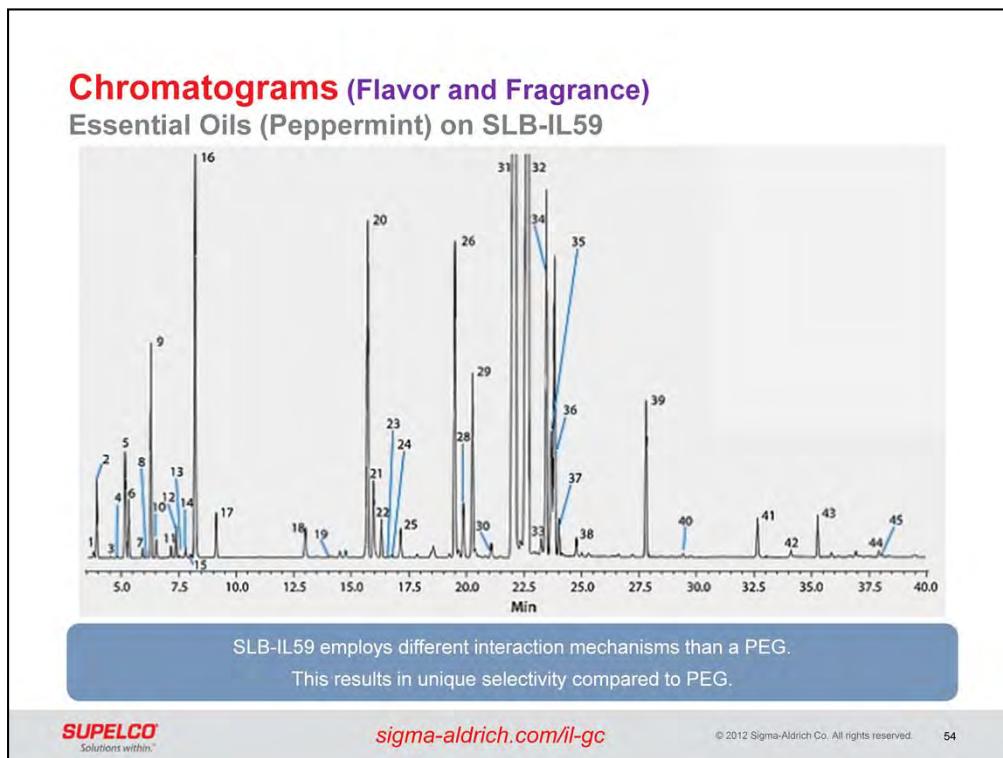
SUPELCO WAX 10 Conditions

- column: SUPELCO WAX 10, 30 m x 0.25 mm I.D., 0.25 μ m (24079)
- oven: 50 $^{\circ}$ C, 5 $^{\circ}$ C/min to 250 $^{\circ}$ C (10 min)
- inj. temp.: 250 $^{\circ}$ C
- detector: FID, 250 $^{\circ}$ C
- carrier gas: helium, 25 cm/sec set at 110 $^{\circ}$ C
- injection: 0.1 μ L, 100:1 split
- liner: 4 mm I.D., split type, cup design
- sample: patchouli essential oil, neat

SLB-IL60 Conditions

- column: SLB-IL60, 30 m x 0.25 mm I.D., 0.20 μ m (29505-U)
- All other conditions the same as those used for the SUPELCO WAX 10

[Chromatogram IDs = G006069 (SUPELCO WAX 10), G006075 (SLB-IL60)]



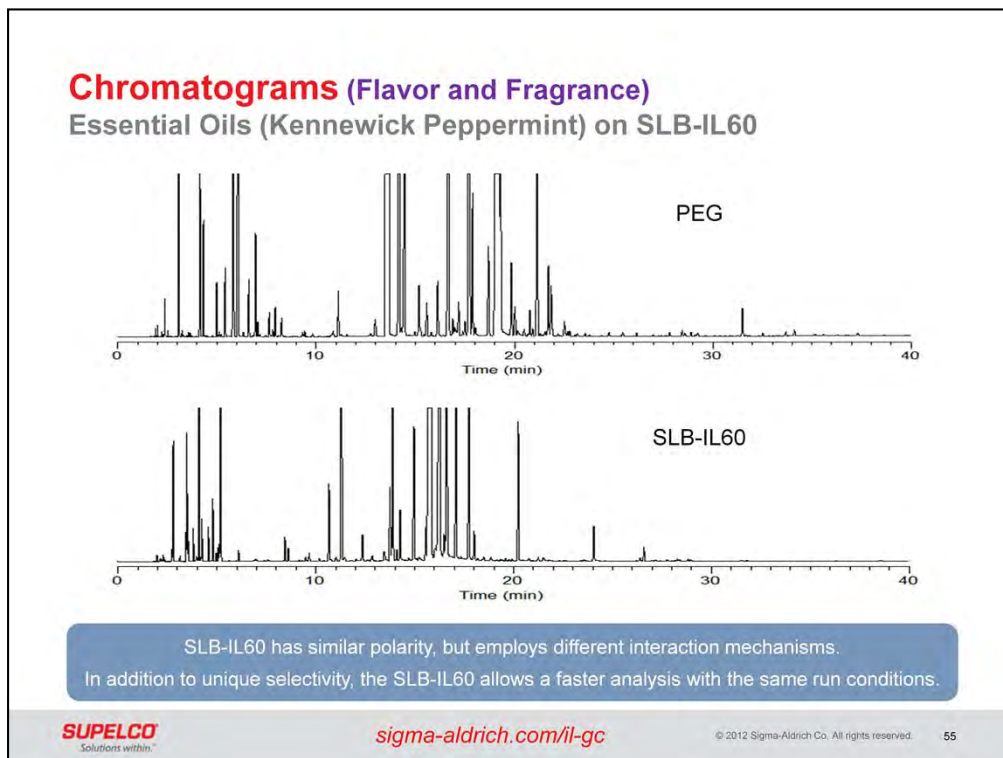
Essential oils are complex mixtures of many compounds. They have different olfactory properties that make some more valuable than others. Smell and taste alone may not be adequate to identify one type from another. GC is a useful tool for performing fingerprinting analysis to identify the type. Columns made with polyethylene glycol (PEG) phases are commonly used. This slide shows the analysis of a peppermint essential oil on a SLB-IL59, which employs different interaction mechanisms than a PEG. This results in unique selectivity compared to PEG.

Chromatogram courtesy of Prof. Luigi Mondello (Univ. of Messina, Italy)

Conditions

- column: SLB-IL59, 30 m x 0.25 mm I.D., 0.20 μm (28891-U)
- oven: 50 $^{\circ}\text{C}$, 3 $^{\circ}\text{C}/\text{min}$ to 300 $^{\circ}\text{C}$
- inj. temp.: 250 $^{\circ}\text{C}$
- detector: MS, scan range m/z 40-400
- carrier gas: helium
- injection: 50:1 split
- liner: wool packed
- sample: peppermint essential oil, diluted 1:10 in hexane

[Chromatogram ID = G005906]



Essential oils are complex mixtures of many compounds. They have different olfactory properties that make some more valuable than others. Smell and taste alone may not be adequate to identify one type from another. GC is a useful tool for performing fingerprinting analysis to identify the type. Columns made with polyethylene glycol (PEG) phases are commonly used. This slide shows the analysis of a Kennewick peppermint essential oil on a PEG and also on a SLB-IL60. The SLB-IL60 has similar polarity, but employs different interaction mechanisms. In addition to unique selectivity, the SLB-IL60 allows a faster analysis with the same run conditions.

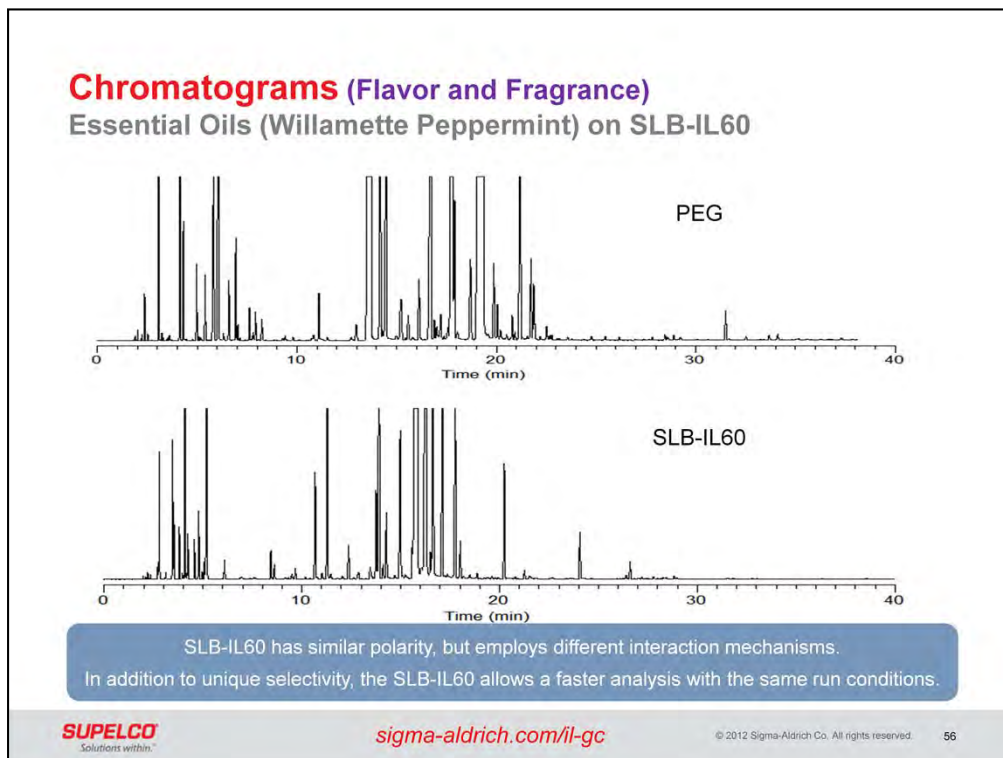
SUPELCO WAX 10 Conditions

- column: SUPELCO WAX 10, 30 m x 0.25 mm I.D., 0.25 μ m (24079)
- oven: 75 $^{\circ}$ C (4 min), 4 $^{\circ}$ C/min to 200 $^{\circ}$ C (10 min)
- inj. temp.: 250 $^{\circ}$ C
- detector: FID, 250 $^{\circ}$ C
- carrier gas: helium, 25 cm/sec set at 110 $^{\circ}$ C
- injection: 0.1 μ L, 100:1 split
- liner: 4 mm I.D., split type, cup design
- sample: Kennewick peppermint essential oil, neat

SLB-IL60 Conditions

- column: SLB-IL60, 30 m x 0.25 mm I.D., 0.20 μ m (29505-U)
- All other conditions the same as those used for the SUPELCO WAX 10

[Chromatogram IDs = G006067 (SUPELCO WAX 10), G006070 (SLB-IL60)]



Essential oils are complex mixtures of many compounds. They have different olfactory properties that make some more valuable than others. Smell and taste alone may not be adequate to identify one type from another. GC is a useful tool for performing fingerprinting analysis to identify the type. Columns made with polyethylene glycol (PEG) phases are commonly used. This slide shows the analysis of a Willamette peppermint essential oil on a PEG and also on a SLB-IL60. The SLB-IL60 has similar polarity, but employs different interaction mechanisms. In addition to unique selectivity, the SLB-IL60 allows a faster analysis with the same run conditions.

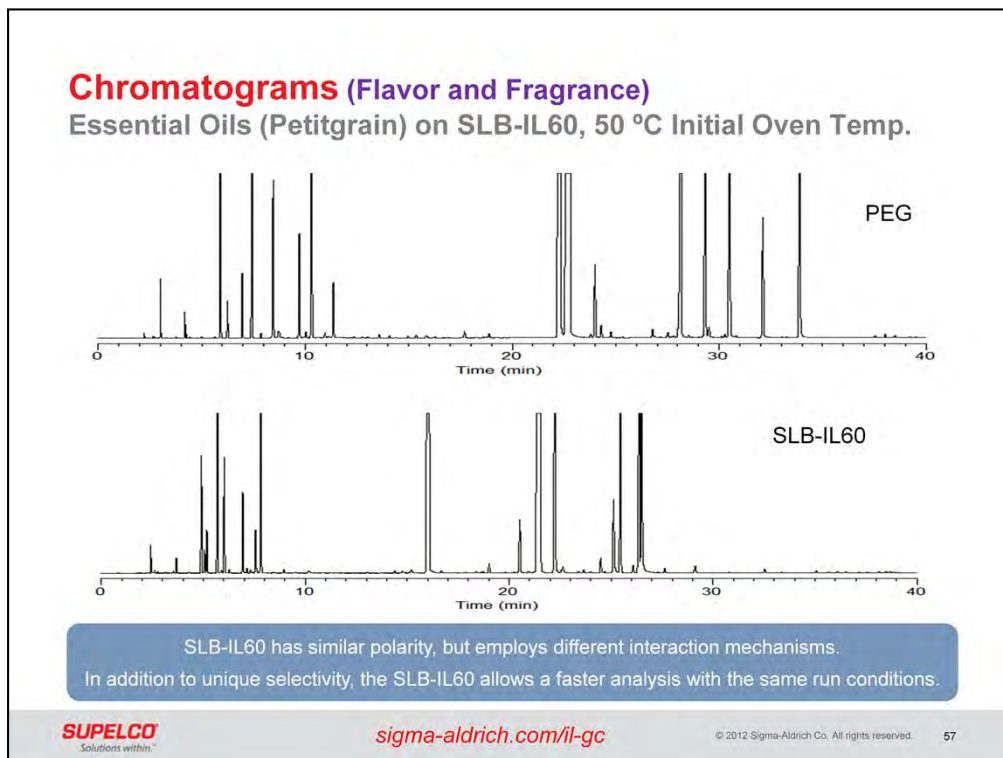
SUPELCO WAX 10 Conditions

- column: SUPELCO WAX 10, 30 m x 0.25 mm I.D., 0.25 μ m (24079)
- oven: 75 $^{\circ}$ C (4 min), 4 $^{\circ}$ C/min to 200 $^{\circ}$ C (10 min)
- inj. temp.: 250 $^{\circ}$ C
- detector: FID, 250 $^{\circ}$ C
- carrier gas: helium, 25 cm/sec set at 110 $^{\circ}$ C
- injection: 0.1 μ L, 100:1 split
- liner: 4 mm I.D., split type, cup design
- sample: Willamette peppermint essential oil, neat

SLB-IL60 Conditions

- column: SLB-IL60, 30 m x 0.25 mm I.D., 0.20 μ m (29505-U)
- All other conditions the same as those used for the SUPELCO WAX 10

[Chromatogram IDs = G006068 (SUPELCO WAX 10), G006071 (SLB-IL60)]



Essential oils are complex mixtures of many compounds. They have different olfactory properties that make some more valuable than others. Smell and taste alone may not be adequate to identify one type from another. GC is a useful tool for performing fingerprinting analysis to identify the type. Columns made with polyethylene glycol (PEG) phases are commonly used. This slide shows the analysis of a petitgrain essential oil on a PEG and also on a SLB-IL60. The SLB-IL60 has similar polarity, but employs different interaction mechanisms. In addition to unique selectivity, the SLB-IL60 allows a faster analysis with the same run conditions.

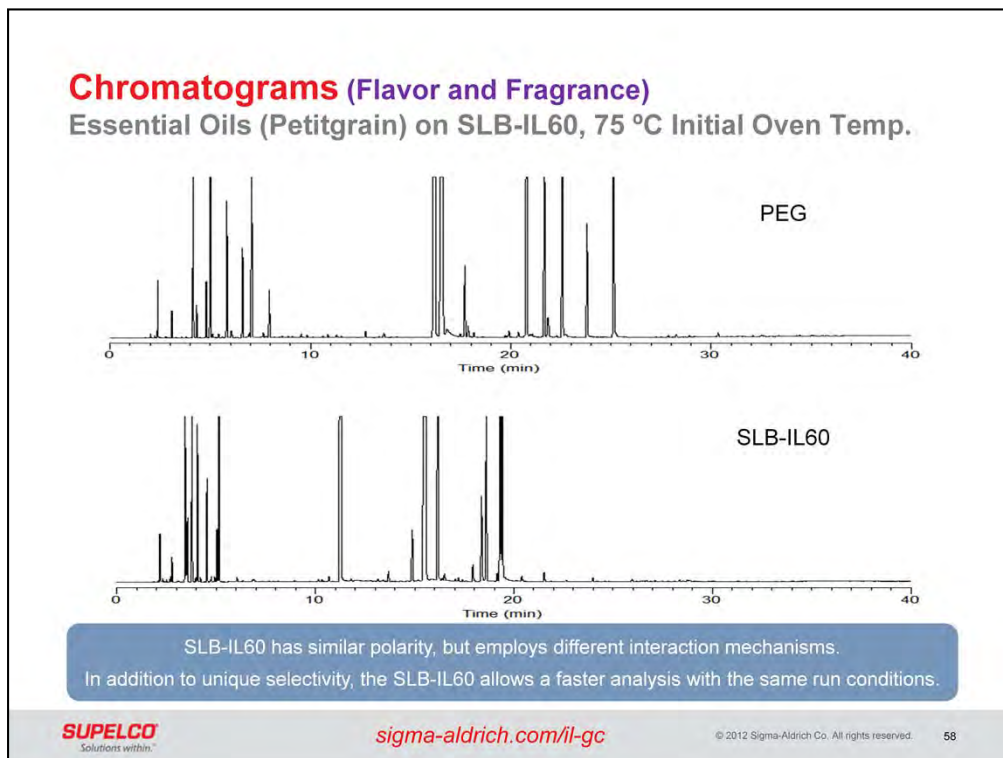
SUPELCO WAX 10 Conditions

- column: SUPELCO WAX 10, 30 m x 0.25 mm I.D., 0.25 μ m (24079)
- oven: 50 °C, 3 °C/min to 250 °C (10 min)
- inj. temp.: 250 °C
- detector: FID, 260 °C
- carrier gas: helium, 25 cm/sec set at 110 °C
- injection: 0.1 μ L, 100:1 split
- liner: 4 mm I.D., split type, cup design
- sample: petitgrain essential oil, neat

SLB-IL60 Conditions

- column: SLB-IL60, 30 m x 0.25 mm I.D., 0.20 μ m (29505-U)
- All other conditions the same as those used for the SUPELCO WAX 10

[Chromatogram IDs = G006077 (SUPELCO WAX 10), G006074 (SLB-IL60)]



Essential oils are complex mixtures of many compounds. They have different olfactory properties that make some more valuable than others. Smell and taste alone may not be adequate to identify one type from another. GC is a useful tool for performing fingerprinting analysis to identify the type. Columns made with polyethylene glycol (PEG) phases are commonly used. This slide shows the analysis of a petitgrain essential oil on a PEG and also on a SLB-IL60. The SLB-IL60 has similar polarity, but employs different interaction mechanisms. In addition to unique selectivity, the SLB-IL60 allows a faster analysis with the same run conditions.

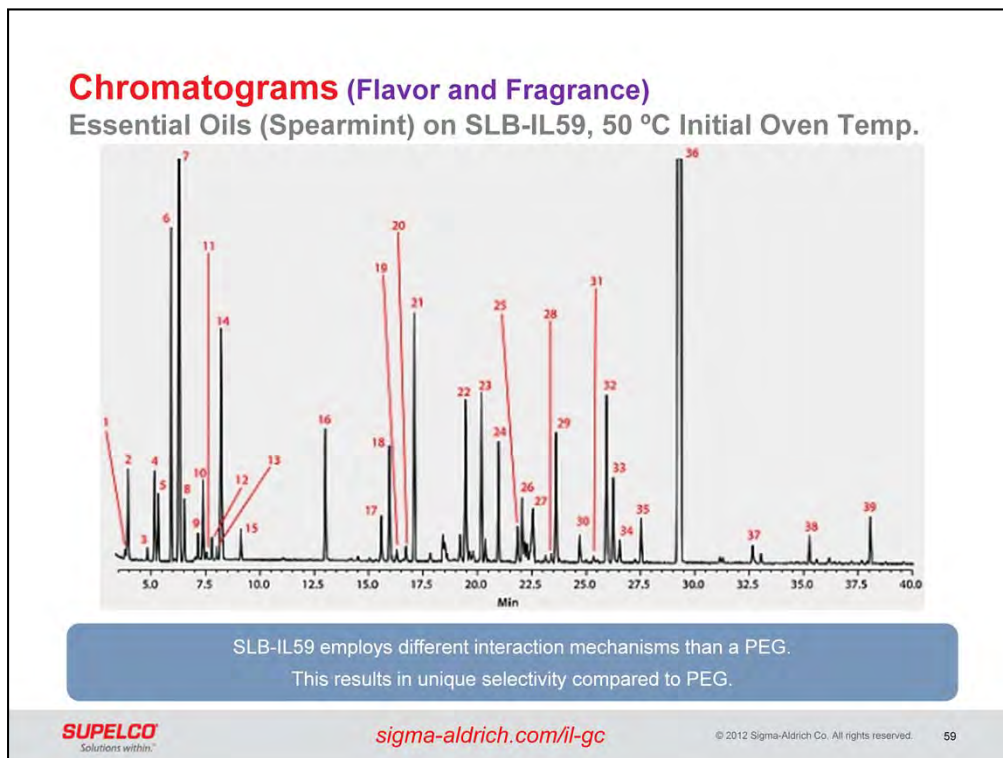
SUPELCO WAX 10 Conditions

- column: SUPELCO WAX 10, 30 m x 0.25 mm I.D., 0.25 μ m (24079)
- oven: 75 °C (4 min), 4 °C/min to 200 °C (10 min)
- inj. temp.: 250 °C
- detector: FID, 250 °C
- carrier gas: helium, 25 cm/sec set at 110 °C
- injection: 0.1 μ L, 100:1 split
- liner: 4 mm I.D., split type, cup design
- sample: petitgrain essential oil, neat

Conditions

- column: SLB-IL60, 30 m x 0.25 mm I.D., 0.20 μ m (29505-U)
- All other conditions the same as those used for the SUPELCO WAX 10

[Chromatogram IDs = G006076 (SUPELCO WAX 10), G006072 (SLB-IL60)]



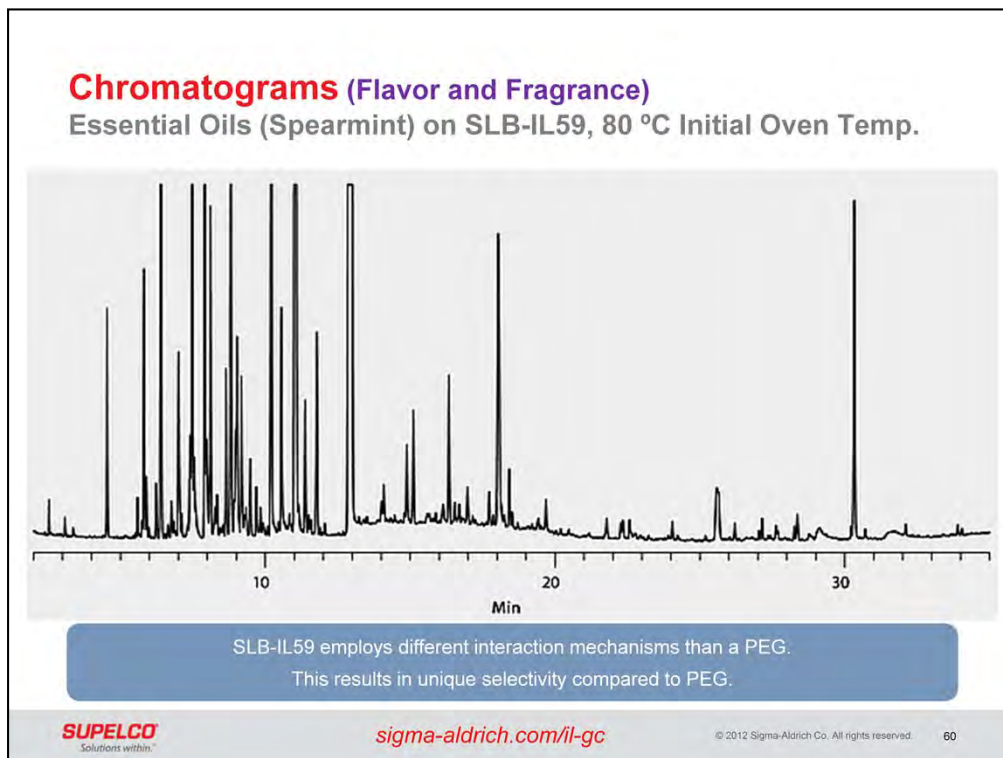
Essential oils are complex mixtures of many compounds. They have different olfactory properties that make some more valuable than others. Smell and taste alone may not be adequate to identify one type from another. GC is a useful tool for performing fingerprinting analysis to identify the type. Columns made with polyethylene glycol (PEG) phases are commonly used. This slide shows the analysis of a spearmint essential oil on a SLB-IL59, which employs different interaction mechanisms than a PEG. This results in unique selectivity compared to PEG.

Chromatogram courtesy of Prof. Luigi Mondello (Univ. of Messina, Italy)

Conditions

- column: SLB-IL59, 30 m x 0.25 mm I.D., 0.20 μ m (28891-U)
- oven: 50 °C, 3 °C/min to 300 °C
- detector: FID
- carrier gas: helium, 30 cm/sec
- sample: spearmint essential oil

[Chromatogram ID = G005898]



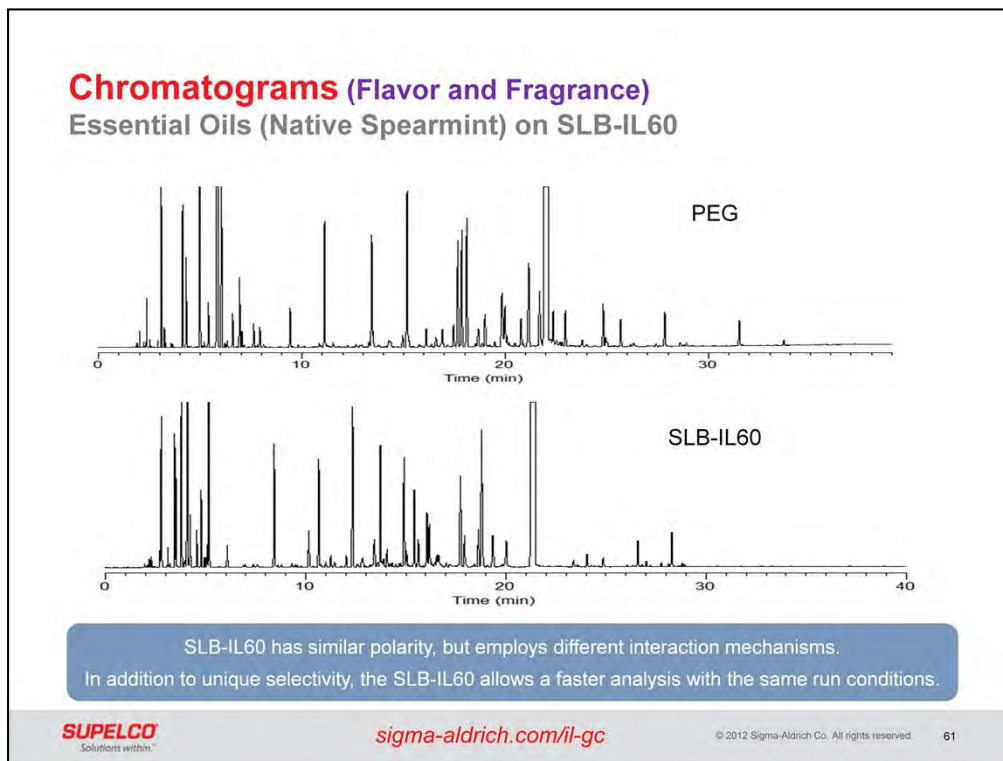
Essential oils are complex mixtures of many compounds. They have different olfactory properties that make some more valuable than others. Smell and taste alone may not be adequate to identify one type from another. GC is a useful tool for performing fingerprinting analysis to identify the type. Columns made with polyethylene glycol (PEG) phases are commonly used. This slide shows the analysis of a spearmint essential oil on a SLB-IL59, which employs different interaction mechanisms than a PEG. This results in unique selectivity compared to PEG.

Chromatogram courtesy of Prof. Luigi Mondello (Univ. of Messina, Italy)

Conditions

- column: SLB-IL59, 30 m x 0.25 mm I.D., 0.20 μ m (28891-U)
- oven: 80 °C, 3 °C/min to 280 °C
- inj. temp.: 250 °C
- detector: FID, 305 °C
- carrier gas: helium, 40 cm/sec
- injection: 1 μ L, 100:1 split
- sample: spearmint essential oil, diluted 1:10 in hexane

[Chromatogram ID = G006066]



Essential oils are complex mixtures of many compounds. They have different olfactory properties that make some more valuable than others. Smell and taste alone may not be adequate to identify one type from another. GC is a useful tool for performing fingerprinting analysis to identify the type. Columns made with polyethylene glycol (PEG) phases are commonly used. This slide shows the analysis of a native spearmint essential oil on a PEG and also on a SLB-IL60. The SLB-IL60 has similar polarity, but employs different interaction mechanisms. In addition to unique selectivity, the SLB-IL60 allows a faster analysis with the same run conditions.

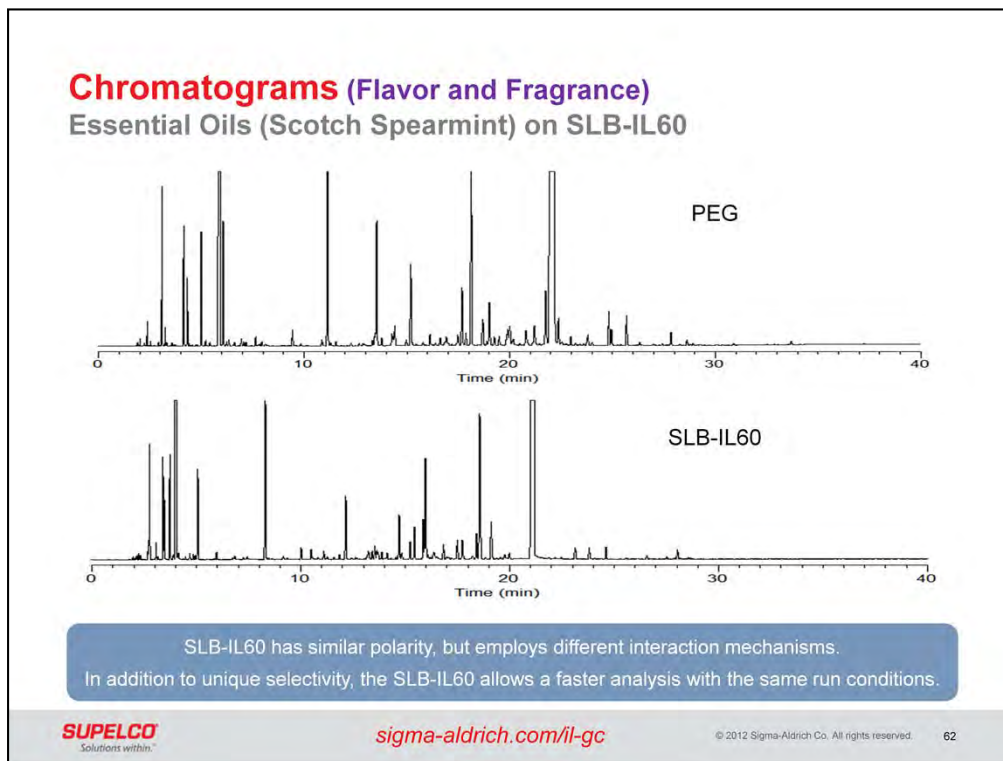
SUPELCO WAX 10 Conditions

- column: SUPELCO WAX 10, 30 m x 0.25 mm I.D., 0.25 μ m (24079)
- oven: 75 $^{\circ}$ C (4 min), 4 $^{\circ}$ C/min to 200 $^{\circ}$ C (10 min)
- inj. temp.: 250 $^{\circ}$ C
- detector: FID, 250 $^{\circ}$ C
- carrier gas: helium, 25 cm/sec set at 110 $^{\circ}$ C
- injection: 0.1 μ L, 100:1 split
- liner: 4 mm I.D., split type, cup design
- sample: native spearmint essential oil, neat

SLB-IL60 Conditions

- column: SLB-IL60, 30 m x 0.25 mm I.D., 0.20 μ m (29505-U)
- All other conditions the same as those used for the SUPELCO WAX 10

[Chromatogram IDs = G006085 (SUPELCO WAX 10), G006083 (SLB-IL60)]



Essential oils are complex mixtures of many compounds. They have different olfactory properties that make some more valuable than others. Smell and taste alone may not be adequate to identify one type from another. GC is a useful tool for performing fingerprinting analysis to identify the type. Columns made with polyethylene glycol (PEG) phases are commonly used. This slide shows the analysis of a scotch spearmint essential oil on a PEG and also on a SLB-IL60. The SLB-IL60 has similar polarity, but employs different interaction mechanisms. In addition to unique selectivity, the SLB-IL60 allows a faster analysis with the same run conditions.

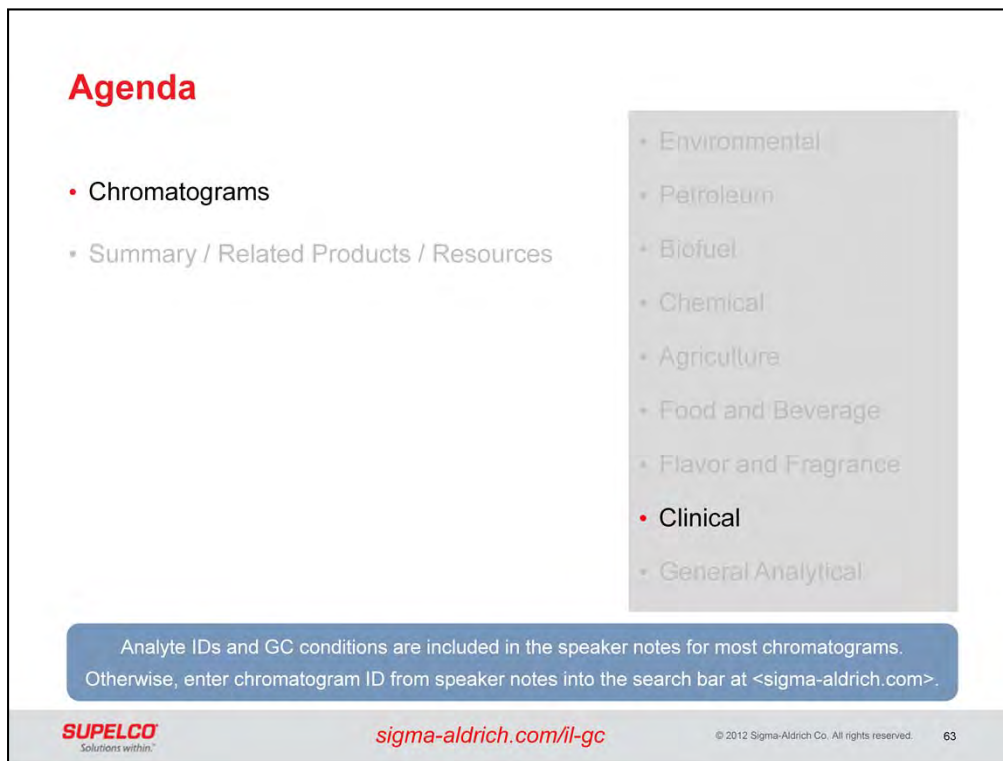
SUPELCOWAX 10 Conditions

- column: SUPELCOWAX 10, 30 m x 0.25 mm I.D., 0.25 μ m (24079)
- oven: 75 $^{\circ}$ C (4 min), 4 $^{\circ}$ C/min to 200 $^{\circ}$ C (10 min)
- inj. temp.: 250 $^{\circ}$ C
- detector: FID, 250 $^{\circ}$ C
- carrier gas: helium, 25 cm/sec set at 110 $^{\circ}$ C
- injection: 0.1 μ L, 100:1 split
- liner: 4 mm I.D., split type, cup design
- sample: scotch spearmint essential oil, neat

SLB-IL60 Conditions

- column: SLB-IL60, 30 m x 0.25 mm I.D., 0.20 μ m (29505-U)
- All other conditions the same as those used for the SUPELCOWAX 10

[Chromatogram IDs = G006086 (SUPELCOWAX 10), G006087 (SLB-IL60)]



Agenda

- Chromatograms
- Summary / Related Products / Resources

- Environmental
- Petroleum
- Biofuel
- Chemical
- Agriculture
- Food and Beverage
- Flavor and Fragrance
- **Clinical**
- General Analytical

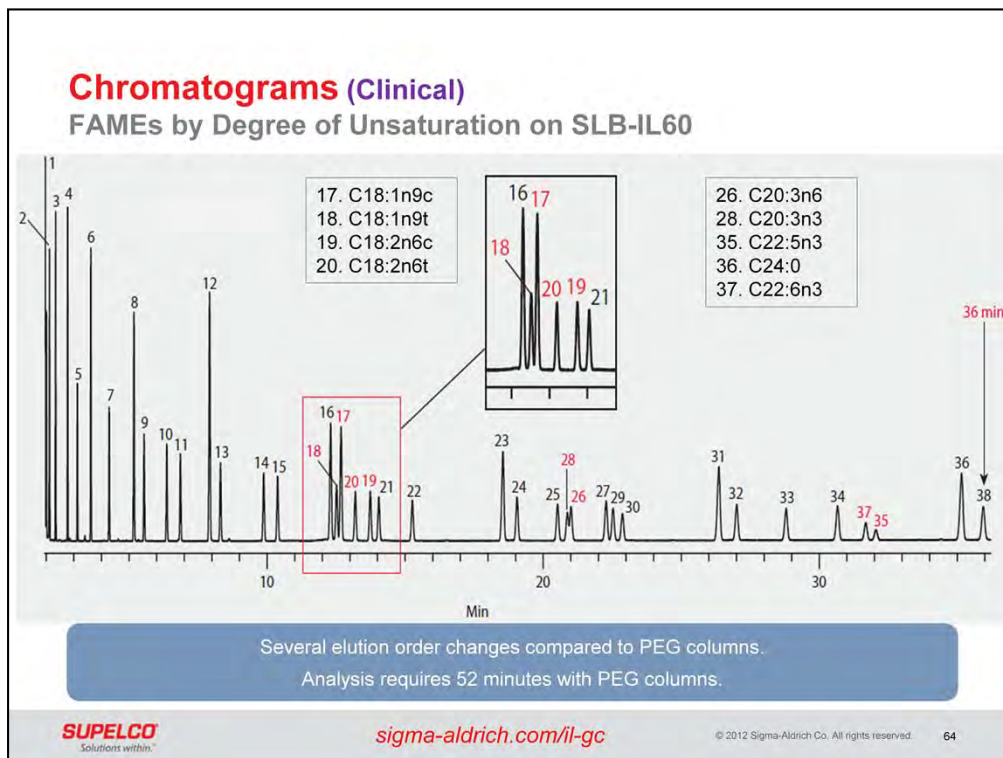
Analyte IDs and GC conditions are included in the speaker notes for most chromatograms. Otherwise, enter chromatogram ID from speaker notes into the search bar at <sigma-aldrich.com>.

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Chromatograms – Clinical Applications

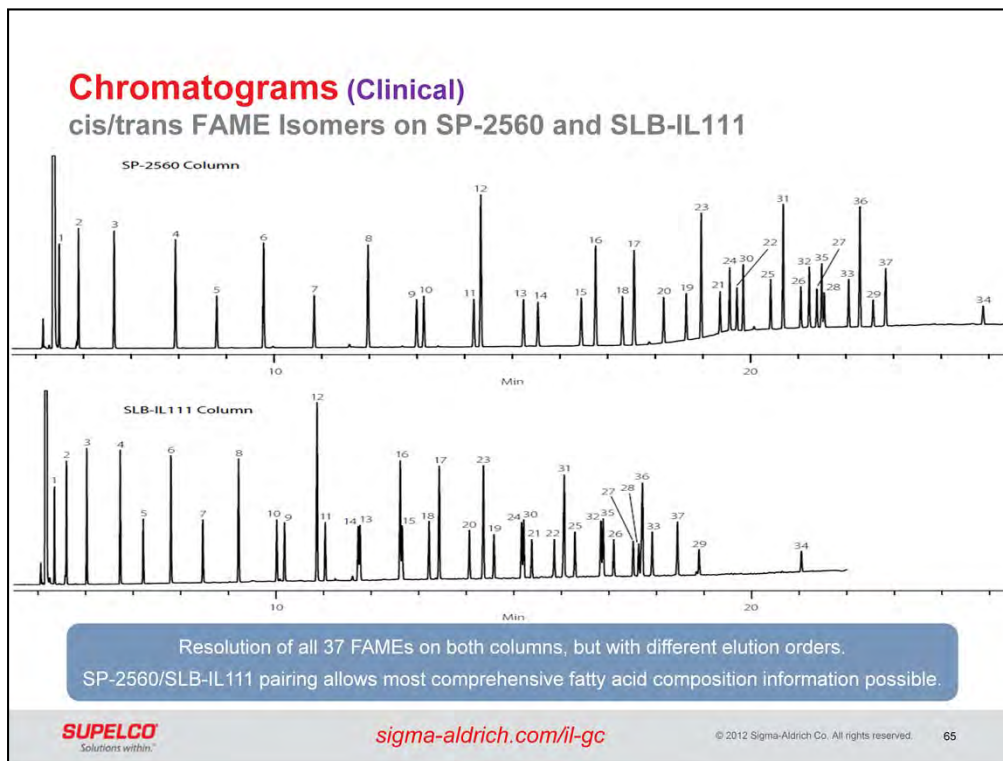


Analyzing FAMES by degree of unsaturation is used to determine the amount of saturated, monounsaturated, and polyunsaturated fats. This chromatogram of C4 to C24 FAMES was analyzed on the SLB-IL60 column. Some interesting elution order changes were noted between the SLB-IL60 and columns made with a polyethylene glycol (PEG) phase. Especially surprising was the elution of C22:6n3 (peak 37) before C22:5n3 (peak 35). Even with one more double bond, it exhibited less retention. Also of note is that this analysis requires 52 minutes with a PEG column. The SLB-IL60 is able to perform this in just 36 minutes.

Conditions

- column: SLB-IL60, 30 m x 0.25 mm I.D., 0.20 μ m (29505-U)
- oven: 170 $^{\circ}$ C, 1 $^{\circ}$ C/min to 225 $^{\circ}$ C
- inj. temp.: 250 $^{\circ}$ C
- detector: FID, 260 $^{\circ}$ C
- carrier gas: helium, 1.2 mL/min
- injection: 1 μ L, 100:1 split
- liner: 4 mm I.D., split/splitless type, single taper wool packed FocusLiner design
- sample: Supelco 37-Component FAME Mix (47885-U) + C22:5n3, in methylene chloride

[Chromatogram ID = G005763]



One indicator of a person's wellness is their fatty acid profile. This involves determining the ratios and amounts of various saturated, monounsaturated, and polyunsaturated fatty acids. This is accomplished by extraction of fatty acids from plasma, conversion to FAMES, and analysis by GC. These chromatograms of C4 to C24 FAMES on the SP-2560 and SLB-IL111 represent the ultimate in FAME analysis. This is because the SP-2560/SLB-IL111 pairing allows the most comprehensive fatty acid composition information possible.

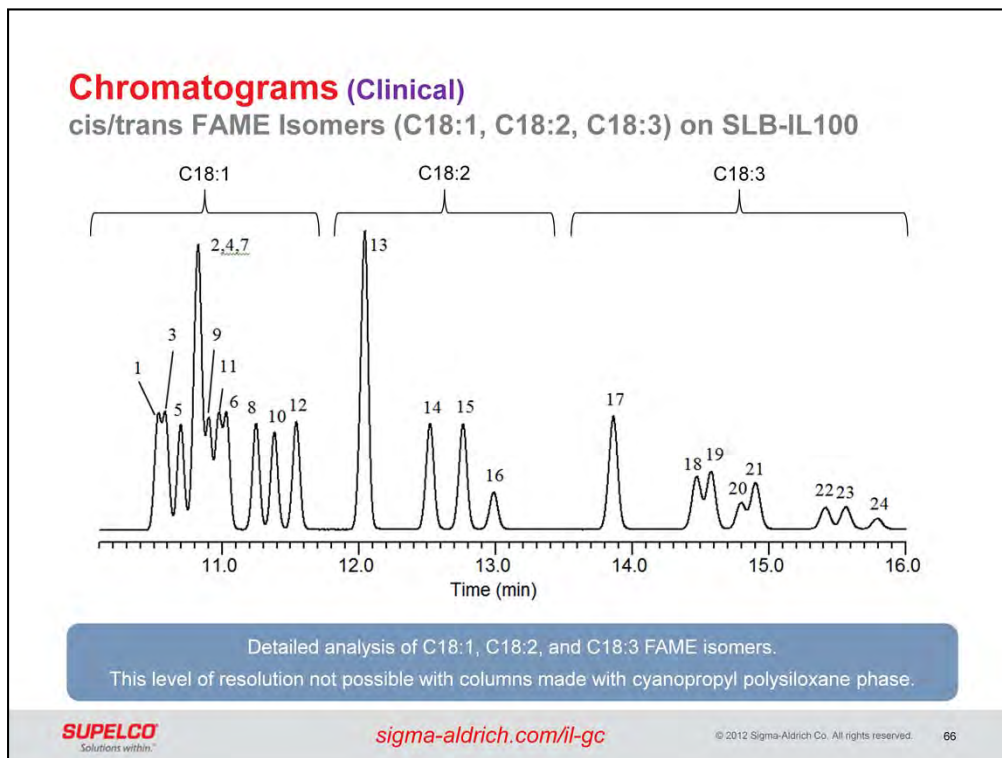
SP-2560 Conditions

- column: SP-2560, 100 m x 0.25 mm I.D., 0.20 μ m (24056)
- oven: 140 $^{\circ}$ C (5 min), 8 $^{\circ}$ C/min to 180 $^{\circ}$ C, 4 $^{\circ}$ C/min to 210 $^{\circ}$ C, 20 $^{\circ}$ C/min to 250 $^{\circ}$ C (7 min)
- inj. temp.: 250 $^{\circ}$ C
- detector: FID, 250 $^{\circ}$ C
- carrier gas: hydrogen, 40 cm/sec
- injection: 1 μ L, 100:1 split
- liner: 4 mm I.D., split type, cup design
- sample: Supelco 37-Component FAME Mix (47885-U)

SLB-IL111 Conditions

- column: SLB-IL111, 100 m x 0.25 mm I.D., 0.20 μ m (29647-U)
- oven: 140 $^{\circ}$ C (5 min), 8 $^{\circ}$ C/min to 180 $^{\circ}$ C, 5 $^{\circ}$ C/min to 260 $^{\circ}$ C
- detector: FID, 260 $^{\circ}$ C
- All other conditions the same as those used for the SP-2560

[Chromatogram IDs = G005366 (SP-2560), G005367 (SLB-IL111)]



In addition to general lipid tests (such as HDL, LDL, and triglycerides), health care providers may also be interested in individual analytes. Trans fatty acids cause adverse health consequences. Some of the most common unsaturated fatty acids are the C18 series. Testing is accomplished by extraction of fatty acids from plasma, conversion to FAMES, and analysis by GC. This chromatogram shows a detailed analysis of C18:1, C18:2, and C18:3 fatty acid isomers, as fatty acid methyl esters (FAMES) on a SLB-IL100. This level of resolution is not possible with columns made with cyanopropyl polysiloxane phase.

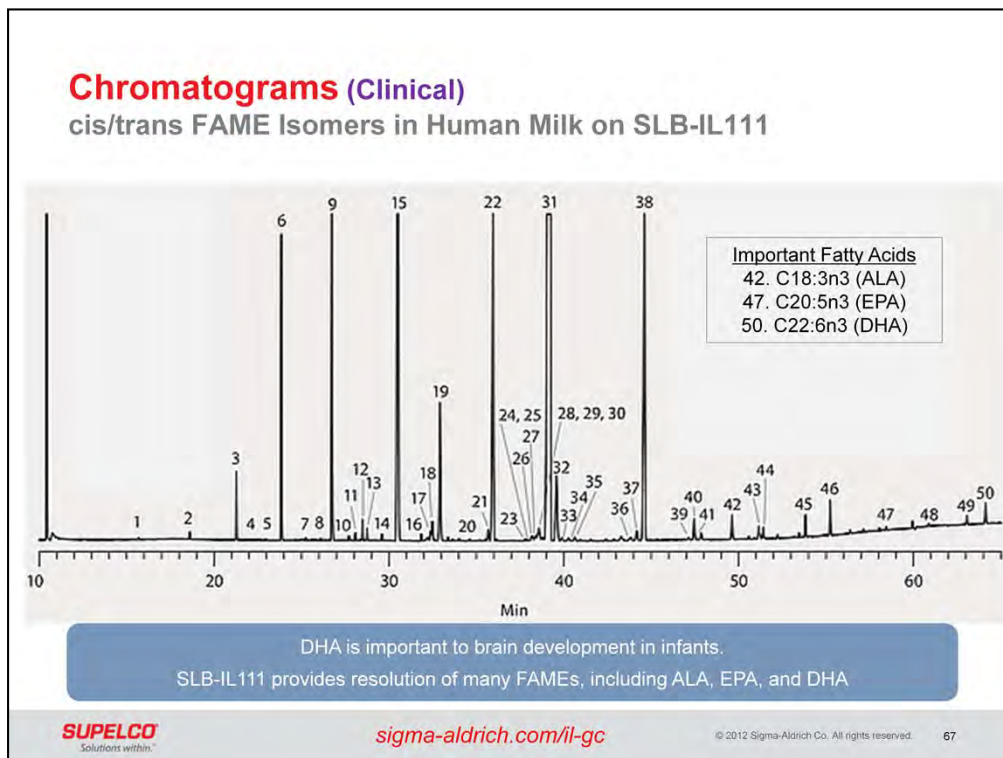
Peak IDs

1. C18:1Δ6t
2. C18:1Δ6c
3. C18:1Δ7t
4. C18:1Δ7c
5. C18:1Δ9t
6. C18:1Δ9c
7. C18:1Δ11t
8. C18:1Δ11c
9. C18:1Δ12t
10. C18:1Δ12c
11. C18:1Δ13t
12. C18:1Δ13c
13. C18:2Δ9t,12t
14. C18:2Δ9c,12t
15. C18:2Δ9t,12c
16. C18:2Δ9c,12c
17. C18:3Δ9t,12t,15t
18. C18:3Δ9t,12t,15c
19. C18:3Δ9t,12c,15t
20. C18:3Δ9c,12c,15t
21. C18:3Δ9c,12t,15t
22. C18:3Δ9c,12t,15c
23. C18:3Δ9t,12c,15c
24. C18:3Δ9c,12c,15c

Conditions

- column: SLB-IL100, 60 m x 0.25 mm I.D., 0.20 μm (28886-U)
- oven: 170 °C
- inj. temp.: 250 °C
- detector: FID, 250 °C
- carrier gas: helium, 30 cm/sec
- injection: 1 μL, 50:1 split
- liner: 4 mm I.D., split type, cup design
- sample: mixture of C18:1, C18:2, and C18:3 FAMES in methylene chloride

[Chromatogram ID = G004386]



Human milk is widely used worldwide for nourishing infants. It contains some important fatty acids, such as alpha-linolenic acid (ALA), eicosapentaenoic acid (EPA), and docosahexaenoic acid (DHA).

- ALA is a precursor to the formation within the body of the essential fatty acids eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA)
- DHA is important to brain development in infants

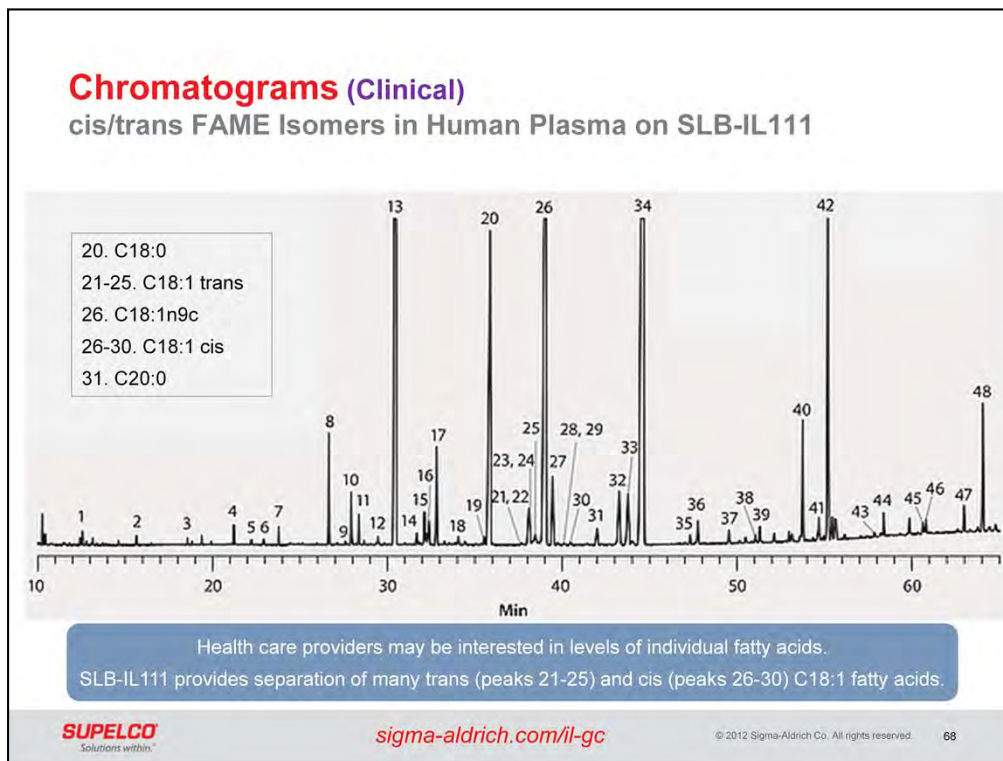
This chromatogram shows FAMEs extracted from human milk on the SLB-IL111. It provides resolution of many FAMEs, including ALA, EPA, and DHA.

Chromatogram courtesy of Prof. Luigi Mondello (Univ. of Messina, Italy)

Conditions

- column: SLB-IL111, 100 m x 0.25 mm I.D., 0.20 μ m (29647-U)
- oven: 50 $^{\circ}$ C (4 min), 8 $^{\circ}$ C/min to 160 $^{\circ}$ C (25 min), 4 $^{\circ}$ C/min to 220 $^{\circ}$ C
- inj. temp.: 230 $^{\circ}$ C
- detector: FID, 240 $^{\circ}$ C
- carrier gas: hydrogen, 40 cm/sec
- injection: 0.2 μ L, 10:1 split
- sample: FAMEs from 100 mg human milk transesterified in sodium methoxide/methanol + boron trifluoride

[Chromatogram ID = G006063]



In addition to general lipid tests (such as HDL, LDL, and triglycerides), health care providers may also be interested in individual analytes. Testing is accomplished by extraction of fatty acids from plasma, conversion to FAMEs, and analysis by GC. This chromatogram shows the analysis of plasma FAMEs on a SLB-IL111, able to provide separation of many trans (peaks 21-25) and cis (peaks 26-30) C18:1 FAMEs.

Chromatogram courtesy of Prof. Luigi Mondello (Univ. of Messina, Italy)

Conditions

- column: SLB-IL111, 100 m x 0.25 mm I.D., 0.20 μ m (29647-U)
- oven: 50 $^{\circ}$ C (4 min), 8 $^{\circ}$ C/min to 160 $^{\circ}$ C (25 min), 4 $^{\circ}$ C/min to 220 $^{\circ}$ C
- inj. temp.: 230 $^{\circ}$ C
- detector: FID, 240 $^{\circ}$ C
- carrier gas: hydrogen, 40 cm/sec
- injection: 2 μ L, 10:1 split
- sample: FAMEs from 500 μ L human plasma transesterified in sodium methoxide/methanol + boron trifluoride

[Chromatogram ID = G006064]

Agenda

- Chromatograms
- Summary / Related Products / Resources

- Environmental
- Petroleum
- Biofuel
- Chemical
- Agriculture
- Food and Beverage
- Flavor and Fragrance
- Clinical
- **General Analytical**

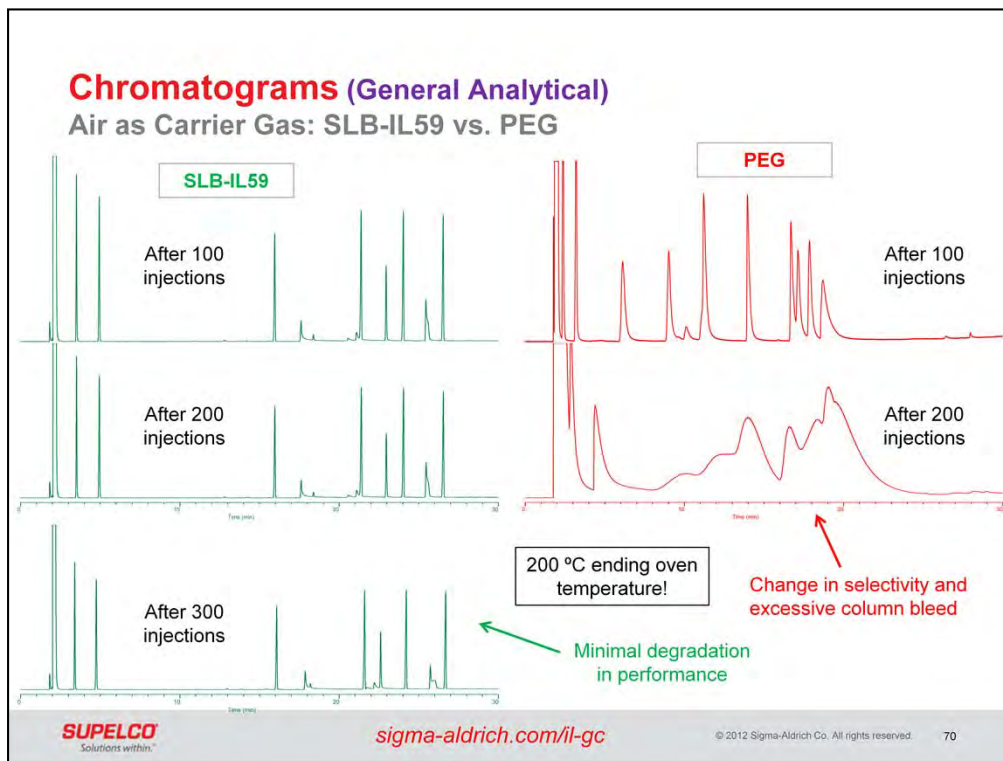
Analyte IDs and GC conditions are included in the speaker notes for most chromatograms. Otherwise, enter chromatogram ID from speaker notes into the search bar at <sigma-aldrich.com>.

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Chromatograms – General Analytical Applications



The active hydroxyl (-OH) groups at the termini of polysiloxane polymer and polyethylene glycol phases make them susceptible to a back-biting reaction, in which polymer fragments are repeatedly cleaved off. This reaction is accelerated by the presence of oxygen or moisture when exposed to heat. Because ionic liquid phases do not possess active hydroxyl groups, they are less susceptible to phase damage under these conditions. This slide shows chromatograms of a test mix on the SLB-IL59 and a PEG using air as the carrier gas. Each column was cycled multiple times through a temperature program of 50 °C to 200 °C. Minimal degradation in performance was observed with the SLB-IL59 column, even after 300 cycles. However, a change in selectivity and excessive column bleed was observed with the PEG column.

SLB-IL59 Conditions

- column: SLB-IL59, 30 m x 0.25 mm I.D., 0.20 µm (28891-U)
- oven: 50 °C (2 min), 4 °C/min to 200 °C (15 min)
- inj. temp.: 250 °C
- detector: 250 °C
- carrier gas: compressed air, 16 psi constant
- injection: 1 µL, 50:1 split
- sample: Programmed Test Mix

PEG Conditions

- column: PEG phase, 30 m x 0.25 mm I.D., 0.25 µm
- All other conditions the same as those used for the SLB-IL59

[Chromatogram ID = G006245]

Agenda

- Chromatograms
- Summary / Related Products / Resources

Summary / Related Products / Resources

Summary

- Something totally new and completely different in the world of GC phases
- Ionic liquids have the opportunity to impact current GC and GC-MS practices along several paths
 - Columns can be engineered with **identical selectivity** to non-ionic liquid columns...
 - *but with higher operating temperatures and less susceptibility to damage from moisture and/or oxygen.*
 - Columns can be engineered with **completely unique selectivity** to non-ionic liquid columns...
 - *producing good peak shape and resolution for compounds of varying functionality.*
 - Columns can be used in **multidimensional separations**...
 - *due to their engineered orthogonality and high thermal stability.*

A wide range of interaction mechanisms translates to different selectivity options.

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Ionic liquids are something totally new and completely different in the world of GC phases. They have the opportunity to impact current GC and GC-MS practices along several paths:

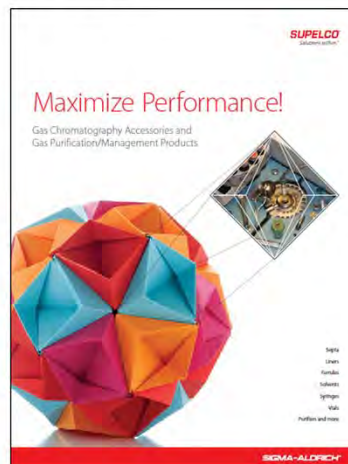
- Columns can be engineered with identical selectivity to non-ionic liquid columns... but with higher operating temperatures and less susceptibility to damage from moisture and/or oxygen
- Columns can be engineered with completely unique selectivity to non-ionic liquid columns... producing good peak shape and resolution for compounds of varying functionality
- Columns can be used in multidimensional separations... due to their engineered orthogonality and high thermal stability

A wide range of interaction mechanisms translates to different selectivity options.

Related Products

Maximize Performance! Brochure (T407103 JWE)

- 28-page, 4-color, bundling brochure
- Lists **common replacement items** (septa, liners, ferrules, solvents, syringes, vials, purifiers, and much more)
- For **several GC makes/models** (Agilent/HP, PerkinElmer, Shimadzu, Thermo, and Varian)



A 'must-have' for all GC labs!

Can be downloaded from <sigma-aldrich.com/gc-learning>.

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There are multiple related products. Most of them are touched on in the 28-page, 4-color Maximize Performance! brochure. This piece lists all the common replacement items, including septa, liners, ferrules, solvents, syringes, vials, purifiers, and much more for several GC makes/models, including Agilent/HP, PerkinElmer, Shimadzu, Thermo, and Varian. This 'must-have' brochure can be downloaded from <sigma-aldrich.com/gc-learning>.


Resources

Complementary Pieces

- “Introduction to the Technology”
 - What are ionic liquid GC columns?
 - How do they relate to non-ionic liquid GC columns and to one another?
 - Selectivity information
 - Details about each phase
- “Bibliography”
 - Peer-reviewed journal articles leading up to and beyond the seminal 2005 JACS (Journal of the American Chemical Society) article
 - Updated periodically

Both pieces can be downloaded from <sigma-aldrich.com/il-gc-lit>.


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There are two complementary pieces. The first is the “Introduction to the Technology” presentation. Topics include:

- What are ionic liquid GC columns?
- How do they relate to non-ionic liquid GC columns and to one another?
- Selectivity information
- Details about each phase

The second is a “Bibliography” of peer-reviewed journal articles leading up to and beyond the seminal 2005 JACS (Journal of the American Chemical Society) article. It is updated periodically.

Both pieces can be downloaded from <sigma-aldrich.com/il-gc-lit>.

Resources

People, Top-Level Literature, and Web Pages

- **Contacts**
 - Marketing (GC Columns): Mike Buchanan <mike.buchanan@sial.com>
 - Marketing (GC Accessories/Gas Purification): Jaime Martain <jaime.martain@sial.com>
 - Technical: Len Sidisky <len.sidisky@sial.com>
- **Brochures**
 - Ionic Liquid GC Columns brochure (planned)
 - Maximize Performance! brochure (T407103 JWE)
- **Web pages (sigma-aldrich.com/il-gc)**
 - Product information
 - Technical literature and application notes
 - Bibliography
 - Request an evaluation

SUPELCO Solutions within.
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Contacts are as follows:

- Marketing for GC Columns is Mike Buchanan
- Marketing for GC Accessories and Gas Purification is Jaime Martain
- Technical is Len Sidisky

An “Ionic Liquid GC Columns” brochure is planned. Use the “Maximize Performance!” brochure for related products.

Visit our ionic liquid landing page to find:

- Detailed product information
- In-depth technical literature and applications notes
- A bibliography of journal articles featuring ionic liquid columns
- A form to request an evaluation column



Thank You