

Prachy... necílený screening s využitím GCxGC HRMS instrumentace

Pavel Jiroš, David E. Alonso and Joe Binkley



How Much a Ruble Is Worth

Note: Scale is inverted to show the decline in the ruble's value.

As of 2:30 p.m. ET





Introduction



"...dust can hold a witch's brew of persistent organic pollutants, metals, endocrine disruptors, and more."

Pelley J., "Dust, Unsettled" ACS Cent. Sci. 2017, 3, 5-9.

- Humans spend a good portion of their time at home (and work)
- Dust is a repository of chemicals and can be used to estimate human exposure to contaminants (e.g., Pesticides, PAHs)

Introduction



Pelley J., "Dust, Unsettled" ACS Cent. Sci. 2017, 3, 5-9.

Name	Formula	R.T. (s)	Similarity	Name	Formula	R.T. (s)	Similarity
Methyl salicylate	$C_8H_8O_3$	688, 2.624	822	Theobromine	$C_7H_8N_4O_2$	2840, 5.155	910
Salicylic acid	$C_7H_6O_3$	840, 3.440	733	Benadryl	$C_{17}H_{21}NO$	2896, 3.345	824
Piperonal	$C_8H_6O_3$	1000, 4.880	919	Musk ketone	$C_{14}H_{18}N_2O_5$	3088, 3.790	809
Nicotine	$C_{10}H_{14}N_2$	1048, 4.085	934	Oxybenzone	$C_{14}H_{12}O_3$	3192, 4.625	873
Vanillin	$C_8H_8O_3$	1208, 6.155	913	Drometrizole	$C_{13}H_{11}N_{3}O$	3272, 4.555	859
Myosmine	$C_9H_{10}N_2$	1328, 7.280	909	Octinoxate	$C_{18}H_{26}O_{3}$	3480, 3.905	883
Lilial	$C_{14}H_{20}O$	1904, 6.620	896	Etocrylene	$C_{18}H_{15}NO_2$	3528, 5.145	763
Diethyltoluamide	$C_{12}H_{17}NO$	2216, 4.055	896	Cocaine	C ₁₇ H ₂₁ NO ₄	3688, 5.255	936
Clorprenaline	$C_{11}H_{16}CINO$	2240, 2.320	781	Padimate O	C ₁₇ H ₂₇ NO ₂	3744, 4.265	879
Ibuprofen	$C_{13}H_{18}O_2$	2328, 2.745	851	Cannabichromene	$C_{21}H_{30}O_2$	4152, 4.500	831
N-Methylsaccharin	$C_8H_7NO_3S$	2360, 3.735	812	Ketazolam	$C_{20}H_{17}CIN_2O_3$	4320, 7.037	785
Acetaminophen	$C_8H_9NO_2$	2488, 3.910	954	Bumetrizole	C ₁₇ H ₁₈ CIN ₃ O	4456, 5.135	725
Veramoss	$C_{10}H_{12}O_4$	2520, 3.027	898	cis-Cinnamoylcocaine	$C_{19}H_{23}NO_4$	4536, 6.305	831
Cotinine	$C_{10}H_{12}N_2O$	2520, 3.830	895	Cannabinol	$C_{21}H_{26}O_2$	4560, 5.332	894
Tolycaine	$C_{15}H_{22}N_2O_3$	2744, 2.635	798	Octocrylene	$C_{24}H_{27}NO_2$	4776, 5.300	849
Caffeine	$C_8H_{10}N_4O_2$	2800, 4.580	903	Octabenzone	$C_{21}H_{26}O_3$	5008, 5.238	835
Tonalid	$C_{18}H_{26}O$	2840, 2.865	842				

- Humans spend a good portion of their time at home (and work)
- Dust is a repository of chemicals and can be used to estimate human ٠ exposure to contaminants (e.g., Pesticides, PAHs)
- Problem: Dust is complex! Numerous, chemically diverse constituents in a wide concentration range

- ✓ Aroma
- ✓ OTC Drugs
- ✓ Illicit Drugs
- ✓ Food/Flavor
- ✓ Tobacco
- ✓ Cannabinoids

Introduction



Pelley J., "Dust, Unsettled" ACS Cent. Sci. 2017, 3, 5-9.

Analytical and Bioanalytical Chemistry https://doi.org/10.1007/s00216-019-01615-6

PAPER IN FOREFRONT



Pawel Rostkowski¹ · Peter Haglund² · Reza Aalizadeh³ · Nikiforos Alygizakis^{3,4} · Nikolaos Thomaidis³ · Joaquin Beltran Arandes⁵ · Pernilla Bohlin Nizzetto¹ · Petra Booij⁶ · Hélène Budzinski⁷ · Pamela Brunswick⁸ · Adrian Covaci⁹ · Christine Gallampois² · Sylvia Grosse¹⁰ · Ralph Hindle¹¹ · Ildiko Ipolyi⁴ · Karl Jobst¹² · Sarit L. Kaserzon¹³ · Pim Leonards¹⁴ · Francois Lestremau¹⁵ · Thomas Letzel¹⁰ · Jörgen Magnér^{16,17} · Hidenori Matsukami¹⁸ · Christoph Moschet¹⁹ · Peter Oswald⁴ · Merle Plassmann²⁰ · Jaroslav Slobodnik⁴ · Chun Yang²¹

updates

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- Humans spend a good portion of their time at home (and work)
- Dust is a repository of chemicals and can be used to estimate human exposure to contaminants (e.g., Pesticides, PAHs)
- Problem: Dust is complex! Numerous, chemically diverse constituents in a wide concentration range
- Analysis of dust has primarily been conducted using targeted methods and a variety of instrumental techniques

Objectives

1) To use a novel multimode source with high resolution time-of-flight mass spectrometry for the non-targeted analysis of dust



Objectives

- 1) To use a novel multimode source with high resolution time-of-flight mass spectrometry for the non-targeted analysis of dust
- 2) To conduct retrospective analysis of the comprehensive data



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- 1) To use a novel multimode source with high resolution time-of-flight mass spectrometry for the non-targeted analysis of dust
- 2) To conduct retrospective analysis of the comprehensive data
- 3) To perform quantitative analysis of Polychlorinated Paraffins (PCPs) in dust



Experimental: Standard & Samples

1) NIST SRM 2585
2) Household Dust
3) Office Dust

Experimental: Compound Extraction



Experimental: Instrument

HRDTM C₂H₅O 1 ppm Mass Accuracy 200 SPECTRA/SECOND

Pegasus HRT+ 4D



Mass Accuracy: 1 PPM Resolution: Up to 50,000 Acquisition Speed: Up to 200 sps Two Sources:

- 1) EI (Dedicated Source)
- 2) Multimode Source (EI, PCI & ECNI)



Part 1 Non-targeted Screening (MMS)





CC C





1st Dimension column: 30m Rxi-5ms (Non-Polar)

Data Processing	Method - "2D Dust MMS RI+2D Dust MMS Classification"		- 🗆 ×
Auto Select	· (🔊 🖬 🕄		
Calibration	Spectral Similarity O Formula O Rev	verse Target 🛛 🔿 Accurate Mass Library	▶ ^
	Enable Spectral Similarity Library Search		
Peak Finding	Maximum Results:	10	
R	Minimum mass to library search:	50	
GCXGC	Maximum mass to library search:	1000	
Subpeak Combining	Minimum molecular weight allowed:	50	
	Maximum molecular weight allowed:	1000	
ON I	Relative abundance threshold (0 - 998):	1	
Target Analyte	Minimum similarity for matches (0 - 999)	500	
Finding	Minimum similarity before bit is assigned (0 - 000).	650	
	Add the likraries to use far ecording below		
Classification	mainlib	Add	
	replib W12rep	Remove	
l 8	W12main	remove	
Spectral Analysis			
668	Column Phase: Semi-Standard Non-Polar V		
Retention Index	Retention Index Filtering		
FF .	Filter by Retention Index:		
	Tolerance 30		
Quantitate Reference	Allow estimated RI substitution for non-polar types		
1.1	Use other non-polar column type data il selected n	on-polar type data is absent	
0 ²	Accurate Mass Filters:		
Annotate Spectral	Filter by molecular ion accurate mass	+/- Mass Window	
Data	Filter by base peak accurate mass	1	
99			
Library	IGS™ Scoring Configuration		
Options	Enable Similarity Check		
	Minimum Similarity for Pass Ration (0 - 999) 800		· ·

Non-targeted Data Processing

- ✓ Peak Find (Deconvolution)
- ✓ Group Classification
- ✓ Database Searches
 - NIST 20,
 - Wiley 12
- ✓ Retention Index Filtering
- ✓ Formula Determinations
 - Mass Accuracy Calculations
 - Molecular, Fragment Ions

Representative Compounds

\checkmark	Hydrocarbons
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- ✓ Acids
- ✓ Aromatics
- ✓ Amines
- ✓ Alcohols
- ✓ Aldehydes
- ✓ Ketones
- ✓ Phenols
- ✓ Terpenes
- ✓ Fatty Acids
- ✓ Sterols
- ✓ Phosphates
- ✓ More...

Benzyl alcoholC ₇ H ₈ O496, 2.064890p-CresolC ₇ H ₈ O520, 2.112826AcetophenoneC ₈ H ₈ O528, 2.143942Phenylethyl AlcoholC ₈ H ₁₀ O576, 2.344884Octanoic acidC ₈ H ₁₆ O ₂ 608, 2.240908Oxazolidin-2-oneC ₃ H ₅ NO ₂ 616, 3.967950Benzenamine, 2-methoxy-C ₁₂ H ₂₄ 648, 1.893917Benzaldehyde, 3,4-dimethyl-C ₉ H ₁₀ O664, 2.592888p-AcetyltolueneC ₉ H ₁₀ O672, 2.678937Methyl salicylateC ₁₀ H ₈ 688, 2.755952Ethanol, 2-phenoxy-C ₁₀ H ₈ O752, 3.504909Nonanoic acidC ₉ H ₁₈ O ₂ 760, 2.6488731-DecanolC ₁₀ H ₂₀ O792, 2.4569201H-Inden-1-one, 2,3-dihydro-C ₈ H ₈ O ₄ 884, 4.076815IndoleC ₉ H ₁₀ O1664, 3.592854SesamolC ₁₀ H ₂₀ O1016, 3.344897SesamolC ₁₀ H ₂₀ O1016, 3.344897Gapric acidC ₁₀ H ₂₀ O1016, 3.344898Benzaldehyde, 4-hydroxy-C ₇ H ₆ O ₃ 1024, 5.354935TopeolinC ₁₀ H ₂₀ O1064, 3.0379222(3H)-Furanone, dihydro-5pentyl-C ₁₀ H ₂₀ O1063, 3.344898Benzaldehyde, 4-hydroxy-C ₇ H ₆ O ₃ 1024, 5.354935TopeolinC ₁₀ H ₂₀ O1064, 3.352864Gapric acidC ₁₀ H ₂₀ O1064, 3.352941 <t< th=""><th>Name</th><th>Formula</th><th>R.T. (s)</th><th>Similarity</th></t<>	Name	Formula	R.T. (s)	Similarity
p-Cresol C ₇ H ₈ O 520, 2.112 826 Acetophenone C ₈ H ₈ O 528, 2.143 942 Phenylethyl Alcohol C ₈ H ₁₀ O 576, 2.344 884 Octanoic acid C ₈ H ₁₆ O ₂ 608, 2.240 908 Oxazolidin-2-one C ₃ H ₅ NO ₂ 616, 3.967 950 Benzenamine, 2-methoxy- C ₁₂ H ₂₄ 648, 1.893 917 Benzaldehyde, 3,4-dimethyl- C ₉ H ₁₀ O 664, 2.592 888 p-Acetyltoluene C ₉ H ₁₀ O 664, 2.592 888 p-Acetyltoluene C ₉ H ₁₀ O 688, 2.632 771 Naphthalene C ₁₀ H ₈ 688, 2.755 952 Ethanol, 2-phenoxy- C ₈ H ₁₀ O ₂ 700, 2.648 809 Benzothiazole C ₁₀ H ₈ 688, 4.076 815 1-Decanol C ₁₀ H ₂₂ O 792, 2.456 920 1H-Inden-1-one, 2,3-dihydro- C ₉ H ₈ O 864, 4.076 815 Indole C ₈ H ₇ N 880,4.418 870 Seamol C ₇ H ₆ O ₃ 912, 4.422	Benzyl alcohol	C ₇ H ₈ O	496, 2.064	890
Acetophenone C 8H80 528, 2.143 942 Phenylethyl Alcohol C 8H100 576, 2.344 884 Octanoic acid C 8H1602 608, 2.240 908 Oxazolidin-2-one C 3H5N02 616, 3.967 950 Benzenamine, 2-methoxy- C 7H9N0 640, 2.768 839 3-Dodecene, (2)- C 12H24 648, 1.893 917 Benzaldehyde, 3,4-dimethyl- C 9H100 664, 2.592 888 p-Acetyltoluene C 9H100 672, 2.678 937 Methyl salicylate C 8H803 688, 2.632 771 Naphthalene C 10H8 688, 2.755 952 Ethanol, 2-phenoxy- C 8H1002 700, 2.648 809 Benzothiazole C 9H1802 760, 2.648 873 1-Decanol C 10H20 792, 2.456 920 IH-Inden-1-one, 2,3-dihydro- C 9H80 864, 4.076 815 Indole C 9H1603 912, 4.422 754 Seamol C 7H00 968, 6.027 854	p-Cresol	C ₇ H ₈ O	520, 2.112	826
Phenylethyl Alcohol C ₈ H ₁₀ O 576, 2.344 884 Octanoic acid C ₈ H ₁₆ O ₂ 608, 2.240 908 Oxazolidin-2-one C ₃ H ₅ NO ₂ 616, 3.967 950 Benzenamine, 2-methoxy- C ₁₂ H ₂₄ 648, 1.893 917 Benzaldehyde, 3,4-dimethyl- C ₉ H ₁₀ O 664, 2.592 888 p-Acetyltoluene C ₉ H ₁₀ O 672, 2.678 937 Methyl salicylate C ₈ H ₈ O ₃ 688, 2.632 771 Naphthalene C ₁₀ H ₈ 688, 2.755 952 Ethanol, 2-phenoxy- C ₈ H ₁₀ O ₂ 720, 3.064 809 Benzothiazole C ₇ H ₅ NS 752, 3.504 909 Nonanoic acid C ₉ H ₁₈ O ₂ 760, 2.648 873 1-Decanol C ₁₀ H ₂₂ O 792, 2.456 920 1H-Inden-1-one, 2,3-dihydro- C ₉ H ₈ O 884, 4.007 815 Indole C ₈ H ₇ N 880, 4.418 870 Sesamol C ₇ H ₆ O ₃ 912, 4.422 754 Benzathydhydro, 1-furaldehyde C ₈ H ₇ N	Acetophenone	C ₈ H ₈ O	528, 2.143	942
Octanoic acid $C_8H_{16}O_2$ $608, 2.240$ 908Oxazolidin-2-one $C_3H_5NO_2$ $616, 3.967$ 950Benzenamine, 2-methoxy- C_7H_9NO $640, 2.768$ 839 3-Dodecene, (Z)- $C_{12}H_{24}$ $648, 1.893$ 917Benzaldehyde, 3,4-dimethyl- $C_9H_{10}O$ $664, 2.592$ 888 p-Acetyltoluene $C_9H_{10}O$ $672, 2.678$ 937 Methyl salicylate $C_8H_8O_3$ $688, 2.632$ 771 Naphthalene $C_{10}H_8$ $688, 2.755$ 952 Ethanol, 2-phenoxy- $C_8H_{10}O_2$ $720, 3.064$ 809 Benzothiazole C_7H_5NS $752, 3.504$ 909 Nonanoic acid $C_9H_8O_2$ $760, 2.648$ 873 1-Decanol $C_{10}H_{2}O$ $792, 2.456$ 920 1H-Inden-1-one, 2,3-dihydro- C_9H_8O $864, 4.076$ 815 Indole C_8H_7N $880, 4.418$ 870 5-Acetoxymethyl-2-furaldehyde $C_8H_8O_4$ $888, 4.200$ 915 Sesamol $C_7H_6O_3$ $912, 4.422$ 754 Benzamide C_7H_7NO $968, 6.027$ 854 Capric acid $C_{10}H_{20}O_2$ $1016, 3.344$ 898 Benzamide, 4-hydroxy- $C_7H_6O_2$ $1024, 5.384$ 935 Topeolin C_8H_7NS $1032, 5.216$ 864 E-11,13-Tetradecadien-1-ol $C_{10}H_{26}O_2$ $1064, 4.352$ 874 1-Tetradecene $C_{12}H_2O_2$ $1064, 4.352$ 901 Acenaphthylene $C_{12}H_2O_2$ $1064,$	Phenylethyl Alcohol	C ₈ H ₁₀ O	576, 2.344	884
Oxazolidin-2-one C ₃ H ₅ NO ₂ 616, 3.967 950 Benzenamine, 2-methoxy- C ₁ H ₉ NO 640, 2.768 839 3-Dodecene, (Z)- C ₁ H ₂₄ 648, 1.893 917 Benzaldehyde, 3,4-dimethyl- C ₉ H ₁₀ O 664, 2.592 888 p-Acetyltoluene C ₉ H ₁₀ O 672, 2.678 937 Methyl salicylate C ₈ H ₈ O ₃ 688, 2.755 952 Ethanol, 2-phenoxy- C ₈ H ₁₀ O 720, 3.064 809 Benzothiazole C ₇ H ₅ NS 752, 3.504 909 Nonanoic acid C ₉ H ₁₈ O 760, 2.648 873 1-Decanol C ₁₀ H ₂₀ 792, 2.456 920 1H-Inden-1-one, 2,3-dihydro- C ₉ H ₈ O 864, 4.076 815 Indole C ₈ H ₇ N 880, 4.418 870 Sesamol C ₇ H ₆ O ₃ 912, 4.422 754 Benzaridehyde, 4-hydroxy- C ₇ H ₆ O ₃ 912, 4.422 754 Capric acid C ₁₀ H ₂₀ O 1008, 3.184 897 Capric acid C ₁₀ H ₂₀ O 10	Octanoic acid	C ₈ H ₁₆ O ₂	608, 2.240	908
Benzenamine, 2-methoxy- $C_{\gamma}H_{9}NO$ $640, 2.768$ 839 3-Dodecene, (Z)- $C_{12}H_{24}$ $648, 1.893$ 917 Benzaldehyde, 3,4-dimethyl- $C_{9}H_{10}O$ $664, 2.592$ 888 p-Acetyltoluene $C_{9}H_{10}O$ $672, 2.678$ 937 Methyl salicylate $C_{8}H_{8}O_{3}$ $688, 2.632$ 7711 Naphthalene $C_{10}H_{8}$ $688, 2.755$ 9522 Ethanol, 2-phenoxy- $C_{8}H_{10}O_{2}$ $720, 3.064$ 809 Benzothiazole $C_{\gamma}H_{5}NS$ $752, 3.504$ 909 Nonanoic acid $C_{9}H_{18}O_{2}$ $760, 2.648$ 873 1-Decanol $C_{10}H_{22}O$ $792, 2.456$ 9201 1H-Inden-1-one, 2,3-dihydro- $C_{9}H_{8}O_{4}$ $880, 4.4076$ 8151 Indole $C_{8}H_{7}N$ $880, 4.418$ 8701 5-Acetoxymethyl-2-furaldehyde $C_{8}H_{8}O_{4}$ $888, 4.200$ 9151 Sesamol $C_{7}H_{6}O_{3}$ $912, 4.422$ 754 Benzanide $C_{2}H_{7}NO$ $968, 6.027$ 854 Capric acid $C_{10}H_{20}O_{2}$ $1008, 3.184$ 8970 Capric acid $C_{10}H_{20}O_{2}$ $1064, 3.037$ 9222 2(3H)-Furanone, dihydro-S-pentyl- $C_{2}H_{10}O_{2}$ $1064, 3.037$ 9222 2(3H)-Furanone, dihydro-S-pentyl- $C_{14}H_{26}O_{2}$ $1064, 3.037$ 9222 2(3H)-Furanone, dihydro-S-pentyl- $C_{12}H_{20}O_{2}$ $1064, 3.037$ 9214 1-Tetradecene $C_{12}H_{20}O_{2}$ $1048, 8.263$ 9011 <td>Oxazolidin-2-one</td> <td>$C_3H_5NO_2$</td> <td>616, 3.967</td> <td>950</td>	Oxazolidin-2-one	$C_3H_5NO_2$	616, 3.967	950
3-Dodecene, (Z)- $C_{12}H_{24}$ 648, 1.893917Benzaldehyde, 3,4-dimethyl- C_9H_{10} O664, 2.592888p-Acetyltoluene C_9H_{10} O672, 2.678937Methyl salicylate $C_8H_8O_3$ 688, 2.632771Naphthalene $C_{10}H_8$ 688, 2.755952Ethanol, 2-phenoxy- $C_8H_{10}O_2$ 720, 3.064809Benzothiazole C_7H_5NS 752, 3.504909Nonanoic acid $C_9H_{18}O_2$ 760, 2.6488731-Decanol $C_{10}H_{20}O$ 792, 2.4569201H-Inden-1-one, 2,3-dihydro- C_9H_8O 864, 4.076815Indole C_8H_7N 880, 4.4188705-Acetoxymethyl-2-furaldehyde $C_8H_8O_4$ 888, 4.200915Sesamol $C_7H_7O_3$ 912, 4.422754Benzanide $C_10H_{20}O_2$ 1008, 3.184897Capric acid $C_{10}H_{20}O_2$ 1064, 3.0379222(3H)-Furanone, dihydro-5-pentyl- $C_9H_6O_2$ 1064, 3.0379222(3H)-Furanone, dihydro-5-pentyl- $C_9H_6O_2$ 1064, 4.3528741-Tetradecene $C_{12}H_2A_0$ 1208, 3.352916Coumarin $C_9H_6O_2$ 1408, 8.263901Acenaphthylene $C_{12}H_2A_0$ 1204, 4.4649001-Dodecanal $C_{12}H_2A_0$ 1504, 4.0689421-Dodecanal $C_{12}H_2A_0$ 1504, 4.4649001-Dodecanalie, N,N-dimethyl- $C_{14}H_{31}N$ 1704, 3.6169421-Dodecanalie,	Benzenamine, 2-methoxy-	C ₇ H ₉ NO	640, 2.768	839
Benzaldehyde, 3,4-dimethyl- $C_9H_{10}O$ $664, 2.592$ 888 p-Acetyltoluene $C_9H_{10}O$ $672, 2.678$ 937 Methyl salicylate $C_8H_8O_3$ $688, 2.632$ 771 Naphthalene $C_{10}H_8$ $688, 2.755$ 952 Ethanol, 2-phenoxy- $C_8H_{10}O_2$ $720, 3.064$ 809 Benzothiazole C_7H_5NS $752, 3.504$ 909 Nonanoic acid $C_9H_{18}O_2$ $760, 2.648$ 873 1-Decanol $C_{10}H_{20}O$ $792, 2.456$ 920 1H-Inden-1-one, 2,3-dihydro- C_9H_8O $864, 4.076$ 815 Indole C_8H_7N $880, 4.418$ 870 5-Acetoxymethyl-2-furaldehyde $C_8H_9O_4$ $888, 4.200$ 915 Sesamol $C_7H_7O_3$ $912, 4.422$ 754 Benzaidehyde, 4-hydroxy- $C_7H_6O_2$ $1008, 3.184$ 897 Capric acid $C_{10}H_{20}O_2$ $1064, 3.037$ 922 2(3H)-Furanone, dihydro-5-pentyl- $C_9H_16O_2$ $1064, 3.037$ 922 2(3H)-Furanone, dihydro-5-pentyl- $C_9H_16O_2$ $1064, 3.037$ 922 2(3H)-Furanone, dihydro-5-pentyl- $C_9H_16O_2$ $1064, 3.037$ 922 2(3H)-Furanone, dihydro-5-pentyl- $C_{14}H_{28}$ $1128, 2.600$ 944 Dodecanal $C_{12}H_2AO$ $1064, 3.037$ 922 2(3H)-Furanone, dihydro-5-pentyl- $C_{14}H_{28}$ $128, 2.630$ 941 Didecanal $C_{12}H_2AO$ $1204, 4.484$ 900 Acenaphthylene $C_{12}H_2AO$ 1204	3-Dodecene, (Z)-	C ₁₂ H ₂₄	648, 1.893	917
p-Acetyltoluene C ₉ H ₁₀ O 672, 2.678 937 Methyl salicylate C ₈ H ₈ O ₃ 688, 2.632 771 Naphthalene C ₁₀ H ₈ 688, 2.755 952 Ethanol, 2-phenoxy- C ₈ H ₁₀ O ₂ 720, 3.064 809 Benzothiazole C ₇ H ₅ NS 752, 3.504 909 Nonanoic acid C ₉ H ₁₈ O ₂ 760, 2.648 873 1-Decanol C ₁₀ H ₂₂ O 792, 2.456 920 1H-Inden-1-one, 2,3-dihydro- C ₉ H ₈ O 864, 4.076 815 Indole C ₈ H ₇ N 880, 4.418 870 5-Acetoxymethyl-2-furaldehyde C ₈ H ₈ O ₄ 888, 4.200 915 Sesamol C ₇ H ₇ NO 968, 6.027 854 Capric acid C ₁₀ H ₂₀ O ₂ 1008, 3.184 897 Capric acid C ₁₀ H ₂₀ O ₂ 1016, 3.344 898 Benzaldehyde, 4-hydroxy- C ₇ H ₆ O ₂ 1024, 5.384 935 Tropeolin C ₈ H ₇ NS 1032, 5.216 864 E-11,13-Tetradecadien-1-01 C ₁₄ H ₂₆ O	Benzaldehyde, 3,4-dimethyl-	C ₉ H ₁₀ O	664, 2.592	888
Methyl salicylate $C_8H_8O_3$ $688, 2.632$ 771 Naphthalene $C_{10}H_8$ $688, 2.755$ 952 Ethanol, 2-phenoxy- $C_8H_{10}O_2$ $720, 3.064$ 809 Benzothiazole C_7H_5NS $752, 3.504$ 909 Nonanoic acid $C_9H_8O_2$ $760, 2.648$ 873 1-Decanol $C_{10}H_{20}O$ $792, 2.456$ 920 1H-Inden-1-one, 2,3-dihydro- C_9H_8O $864, 4.076$ 815 Indole C_8H_7N $880, 4.418$ 870 5-Acetoxymethyl-2-furaldehyde $C_8H_8O_4$ $888, 4.200$ 915 Sesamol $C_7H_6O_3$ $912, 4.422$ 754 Benzamide C_7H_7NO $968, 6.027$ 854 Capric acid $C_10H_{20}O_2$ $1008, 3.184$ 897 Capric acid $C_{10}H_{20}O_2$ $1016, 3.344$ 898 Benzaldehyde, 4-hydroxy- $C_7H_6O_2$ $1024, 5.384$ 935 Tropeolin C_8H_7NS $1032, 5.216$ 864 E-11,13-Tetradecadien-1-ol $C_{14}H_{26}O$ $1064, 4.303$ 922 2(3H)-Furanone, dihydro-5-pentyl- $C_9H_6O_2$ $1064, 4.352$ 916 Oudecanal $C_{12}H_{24}O$ $1408, 8.263$ 901 Acenaphthylene $C_{12}H_{26}O$ $1408, 8.263$ 901 Acenaphthylene $C_{12}H_{20}O_4$ $1624, 4.464$ 900 1-Dodecanol $C_{12}H_{20}O_4$ $1624, 4.464$ 900 1-Dodecanaline, N,N-dimethyl- $C_{14}H_{31}N$ $1744, 4.485$ 890 1-bodecanaline, N,N-di	p-Acetyltoluene	C ₉ H ₁₀ O	672, 2.678	937
Naphthalene $C_{10}H_8$ $688, 2.755$ 952 Ethanol, 2-phenoxy- $C_8H_{10}O_2$ $720, 3.064$ 809 Benzothiazole C_7H_5NS $752, 3.504$ 909 Nonanoic acid $C_9H_{18}O_2$ $760, 2.648$ 873 1-Decanol $C_{10}H_{20}O$ $792, 2.456$ 920 1H-Inden-1-one, 2,3-dihydro- C_9H_8O $864, 4.076$ 815 Indole C_8H_7N $880, 4.418$ 870 5-Acetoxymethyl-2-furaldehyde $C_8H_8O_4$ $888, 4.200$ 915 Sesamol $C_7H_6O_3$ $912, 4.422$ 754 Benzamide C_7H_7NO $968, 6.027$ 854 Capric acid $C_{10}H_{20}O_2$ $1008, 3.184$ 897 Capric acid $C_{10}H_{20}O_2$ $1016, 3.344$ 898 Benzaldehyde, 4-hydroxy- $C_7H_6O_2$ $1024, 5.384$ 935 Tropeolin C_8H_7NS $1032, 5.216$ 864 E-11,13-Tetradecadien-1-ol $C_{14}H_{26}O$ $1064, 4.303$ 922 2(3H)-Furanone, dihydro-5-pentyl- $C_9H_6O_2$ $1064, 4.352$ 874 Dodecanal $C_{12}H_{20}O_4$ $1428, 2.600$ 944 Dodecanal $C_{12}H_{20}O_4$ $1472, 6.872$ 925 1-Dodecanol $C_{12}H_{20}O_4$ $1624, 4.464$ 900 1-Dodecanol $C_{12}H_{20}O_4$ $1624, 4.464$ 900 1-Dodecanaline, N,N-dimethyl- $C_{14}H_{21}N$ $1744, 4.485$ 890 Liuric acid $C_{12}H_{20}O_2$ $1204, 4.008$ 942	Methyl salicylate	C ₈ H ₈ O ₃	688, 2.632	771
Ethanol, 2-phenoxy- $C_8H_{10}O_2$ 720, 3.064809Benzothiazole C_7H_5NS 752, 3.504909Nonanoic acid $C_9H_{18}O_2$ 760, 2.6488731-Decanol $C_{10}H_{22}O$ 792, 2.4569201H-Inden-1-one, 2,3-dihydro- C_9H_8O 864, 4.076815Indole C_8H_7N 880, 4.4188705-Acetoxymethyl-2-furaldehyde $C_8H_8O_4$ 888, 4.200915Sesamol $C_7H_6O_3$ 912, 4.422754Benzamide $C_1H_{20}O_2$ 1008, 3.184897Capric acid $C_{10}H_{20}O_2$ 1016, 3.344898Benzaldehyde, 4-hydroxy- $C_7H_6O_2$ 1024, 5.384935Tropeolin C_8H_7NS 1032, 5.216864E-11,13-Tetradecadien-1-ol $C_{14}H_{26}O$ 1064, 3.0379222(3H)-Furanone, dihydro-5-pentyl- $C_9H_6O_2$ 1064, 3.352916Oudecanal $C_{12}H_{24}O$ 1208, 3.352916Coumarin $C_{12}H_{26}O$ 1504, 4.008954Diisobutyl maleate $C_{12}H_{20}O_4$ 1624, 4.4649001-Dodecanaline, N,N-dimethyl- $C_{14}H_{31}N$ 1704, 3.616942Tridecanal $C_{12}H_{20}O_4$ 1624, 4.468890	Naphthalene	C ₁₀ H ₈	688, 2.755	952
Benzothiazole C_7H_5NS $752, 3.504$ 909Nonanoic acid $C_9H_{18}O_2$ $760, 2.648$ 873 1-Decanol $C_{10}H_{22}O$ $792, 2.456$ 920 1H-Inden-1-one, 2,3-dihydro- C_9H_8O $864, 4.076$ 815 Indole C_8H_7N $880, 4.418$ 870 5-Acetoxymethyl-2-furaldehyde $C_8H_8O_4$ $888, 4.200$ 915 Sesamol $C_7H_6O_3$ $912, 4.422$ 754 Benzamide C_7H_7NO $968, 6.027$ 854 Capric acid $C_{10}H_{20}O_2$ $1008, 3.184$ 897 Capric acid $C_{10}H_{20}O_2$ $1016, 3.344$ 898 Benzaldehyde, 4-hydroxy- $C_7H_6O_2$ $1024, 5.384$ 935 Tropeolin C_8H_7NS $1032, 5.216$ 864 E-11,13-Tetradecadien-1-ol $C_{14}H_{26}O$ $1064, 4.352$ 874 1-Tetradecene $C_{14}H_{26}O$ $1064, 4.352$ 916 Coumarin $C_9H_6O_2$ $1408, 8.263$ 901 Acenaphthylene $C_{12}H_{26}O$ $1504, 4.008$ 954 Diisobutyl maleate $C_{12}H_{20}O_4$ $1624, 4.464$ 900 1-Dodecanaline, N,N-dimethyl- $C_{14}H_{31}N$ $1704, 3.616$ 942 Tridecanal $C_{12}H_{26}O_2$ $1504, 4.085$ 890	Ethanol, 2-phenoxy-	C ₈ H ₁₀ O ₂	720, 3.064	809
Nonanoic acid $C_9H_{18}O_2$ 760, 2.6488731-Decanol $C_{10}H_{22}O$ 792, 2.4569201H-Inden-1-one, 2,3-dihydro- C_9H_8O 864, 4.076815Indole C_8H_7N 880, 4.4188705-Acetoxymethyl-2-furaldehyde $C_8H_8O_4$ 888, 4.200915Sesamol $C_7H_6O_3$ 912, 4.422754Benzamide C_7H_7NO 968, 6.027854Capric acid $C_{10}H_{20}O_2$ 1008, 3.184897Capric acid $C_{10}H_{20}O_2$ 1016, 3.344898Benzaldehyde, 4-hydroxy- $C_7H_6O_2$ 1024, 5.384935Tropeolin C_8H_7NS 1032, 5.216864E-11,13-Tetradecadien-1-ol $C_{14}H_{26}O$ 1064, 3.0379222(3H)-Furanone, dihydro-5-pentyl- $C_9H_6O_2$ 1064, 4.352874Dodecanal $C_{12}H_2AO$ 1208, 3.352916Coumarin $C_9H_6O_2$ 1408, 8.263901Acenaphthylene $C_{12}H_8$ 1472, 6.8729251-Dodecanol $C_{12}H_{20}O_4$ 1624, 4.4649001-Dodecanaline, N,N-dimethyl- $C_{14}H_{31}N$ 1704, 3.616942Tridecanal $C_{12}H_{20}O_4$ 1624, 4.465890Lauric acid $C_{12}H_{20}O_2$ 2120, 4.040906	Benzothiazole	C ₇ H₅NS	752, 3.504	909
1-Decanol $C_{10}H_{20}$ 792, 2.4569201H-Inden-1-one, 2,3-dihydro- C_9H_8O 864, 4.076815Indole C_8H_7N 880, 4.4188705-Acetoxymethyl-2-furaldehyde $C_8H_8O_4$ 888, 4.200915Sesamol $C_7H_6O_3$ 912, 4.422754Benzamide C_7H_7NO 968, 6.027854Capric acid $C_{10}H_{20}O_2$ 1008, 3.184897Capric acid $C_{10}H_{20}O_2$ 1016, 3.344898Benzaldehyde, 4-hydroxy- $C_7H_6O_2$ 1024, 5.384935Tropeolin C_8H_7NS 1032, 5.216864E-11,13-Tetradecadien-1-ol $C_{14}H_{26}O$ 1064, 3.0379222(3H)-Furanone, dihydro-5-pentyl- $C_9H_6O_2$ 1064, 4.352874Dodecanal $C_{12}H_2A$ 1208, 3.352916Coumarin $C_9H_6O_2$ 1408, 8.263901Acenaphthylene $C_{12}H_8$ 1472, 6.8729251-Dodecanol $C_{12}H_{20}O_4$ 1624, 4.4649001-Dodecanaline, N,N-dimethyl- $C_{14}H_{31}N$ 1704, 3.616942Tridecanal $C_{12}H_{20}O_4$ 1624, 4.465890	Nonanoic acid	$C_9H_{18}O_2$	760, 2.648	873
1H-Inden-1-one, 2,3-dihydro- C_9H_8O 864, 4.076815Indole C_8H_7N 880, 4.4188705-Acetoxymethyl-2-furaldehyde $C_8H_8O_4$ 888, 4.200915Sesamol $C_7H_6O_3$ 912, 4.422754Benzamide C_7H_7NO 968, 6.027854Capric acid $C_{10}H_{20}O_2$ 1008, 3.184897Capric acid $C_{10}H_{20}O_2$ 1016, 3.344898Benzaldehyde, 4-hydroxy- $C_7H_6O_2$ 1024, 5.384935Tropeolin C_8H_7NS 1032, 5.216864E-11,13-Tetradecadien-1-0I $C_{14}H_{26}O$ 1064, 3.0379222(3H)-Furanone, dihydro-5-pentyl- $C_9H_16O_2$ 1064, 3.352916Odecanal $C_{12}H_2A$ 1208, 3.352916Coumarin $C_9H_6O_2$ 1408, 8.263901Acenaphthylene $C_{12}H_2A$ 1504, 4.008954Diisobutyl maleate $C_{12}H_{20}O_4$ 1624, 4.4649001-Dodecanaline, N,N-dimethyl- $C_{14}H_{31}N$ 1704, 3.616942Tridecanal $C_{12}H_{20}O_2$ 2120, 4.040906	1-Decanol	C ₁₀ H ₂₂ O	792, 2.456	920
Indole C_8H_7N 880, 4.4188705-Acetoxymethyl-2-furaldehyde $C_8H_8O_4$ 888, 4.200915Sesamol $C_7H_6O_3$ 912, 4.422754Benzamide C_7H_7NO 968, 6.027854Capric acid $C_{10}H_{20}O_2$ 1008, 3.184897Capric acid $C_{10}H_{20}O_2$ 1016, 3.344898Benzaldehyde, 4-hydroxy- $C_7H_6O_2$ 1024, 5.384935Tropeolin C_8H_7NS 1032, 5.216864E-11,13-Tetradecadien-1-0l $C_{14}H_{26}O$ 1064, 3.0379222(3H)-Furanone, dihydro-5-pentyl- $C_9H_16O_2$ 1064, 4.3528741-Tetradecene $C_{12}H_2A$ 128, 2.600944Dodecanal $C_{12}H_2A$ 1208, 3.352916Coumarin $C_9H_6O_2$ 1408, 8.263901Acenaphthylene $C_{12}H_2A$ 1504, 4.008954Diisobutyl maleate $C_{12}H_{20}O_4$ 1624, 4.4649001-Dodecanaline, N,N-dimethyl- $C_{14}H_{31}N$ 1704, 3.616942Tridecanal $C_{12}H_{20}O_2$ 2120, 4.040906	1H-Inden-1-one, 2,3-dihydro-	C ₉ H ₈ O	864, 4.076	815
5-Acetoxymethyl-2-furaldehyde $C_8H_8O_4$ 888, 4.200915Sesamol $C_7H_6O_3$ 912, 4.422754Benzamide C_7H_7NO 968, 6.027854Capric acid $C_{10}H_{20}O_2$ 1008, 3.184897Capric acid $C_{10}H_{20}O_2$ 1016, 3.344898Benzaldehyde, 4-hydroxy- $C_7H_6O_2$ 1024, 5.384935Tropeolin C_8H_7NS 1032, 5.216864E-11,13-Tetradecadien-1-ol $C_{14}H_{26}O$ 1064, 3.0379222(3H)-Furanone, dihydro-5-pentyl- $C_9H_16O_2$ 1064, 4.352874Dodecanal $C_{12}H_{24}O$ 1208, 3.352916Coumarin $C_9H_6O_2$ 1408, 8.263901Acenaphthylene $C_{12}H_8$ 1472, 6.8729251-Dodecanol $C_{12}H_{20}O_4$ 1624, 4.4649001-Dodecanaline, N,N-dimethyl- $C_{14}H_{31}N$ 1704, 3.616942Tridecanal $C_{13}H_{26}O$ 1744, 4.485890	Indole	C ₈ H ₇ N	880, 4.418	870
Sesamol $C_7H_6O_3$ 912, 4.422754Benzamide C_7H_7NO 968, 6.027854Capric acid $C_{10}H_{20}O_2$ 1008, 3.184897Capric acid $C_{10}H_{20}O_2$ 1016, 3.344898Benzaldehyde, 4-hydroxy- $C_7H_6O_2$ 1024, 5.384935Tropeolin C_8H_7NS 1032, 5.216864E-11,13-Tetradecadien-1-ol $C_{14}H_{26}O$ 1064, 3.0379222(3H)-Furanone, dihydro-5-pentyl- $C_9H_16O_2$ 1064, 4.352874Dodecanal $C_{12}H_{24}O$ 1208, 3.352916Coumarin $C_9H_6O_2$ 1408, 8.263901Acenaphthylene $C_{12}H_{26}O$ 1504, 4.008954Diisobutyl maleate $C_{12}H_{20}O_4$ 1624, 4.4649001-Dodecanaline, N,N-dimethyl- $C_{14}H_{31}N$ 1704, 3.616942Tridecanal $C_{12}H_{26}O$ 1204, 4.485890Lauric acid $C_{12}H_{20}O_2$ 2120, 4.040906	5-Acetoxymethyl-2-furaldehyde	C ₈ H ₈ O ₄	888, 4.200	915
Benzamide C_7H_7NO 968, 6.027854Capric acid $C_{10}H_{20}O_2$ 1008, 3.184897Capric acid $C_{10}H_{20}O_2$ 1016, 3.344898Benzaldehyde, 4-hydroxy- $C_7H_6O_2$ 1024, 5.384935Tropeolin C_8H_7NS 1032, 5.216864E-11,13-Tetradecadien-1-0l $C_{14}H_{26}O$ 1064, 3.0379222(3H)-Furanone, dihydro-5-pentyl- $C_9H_16O_2$ 1064, 4.352874Dodecanal $C_{12}H_2AO$ 1208, 3.352916Coumarin $C_9H_6O_2$ 1408, 8.263901Acenaphthylene $C_{12}H_8$ 1472, 6.8729251-Dodecanol $C_{12}H_{20}O_4$ 1624, 4.4649001-Dodecanaline, N,N-dimethyl- $C_{14}H_{31}N$ 1704, 3.616942Tridecanal $C_{12}H_{20}O_2$ 2120, 4.040906	Sesamol	$C_7H_6O_3$	912, 4.422	754
Capric acid $C_{10}H_{20}O_2$ 1008, 3.184897Capric acid $C_{10}H_{20}O_2$ 1016, 3.344898Benzaldehyde, 4-hydroxy- $C_7H_6O_2$ 1024, 5.384935Tropeolin C_8H_7NS 1032, 5.216864E-11,13-Tetradecadien-1-0l $C_{14}H_{26}O$ 1064, 3.0379222(3H)-Furanone, dihydro-5-pentyl- $C_9H_16O_2$ 1064, 4.3528741-Tetradecene $C_{14}H_{28}$ 1128, 2.600944Dodecanal $C_{12}H_2AO$ 1208, 3.352916Coumarin $C_9H_6O_2$ 1408, 8.263901Acenaphthylene $C_{12}H_8$ 1472, 6.8729251-Dodecanol $C_{12}H_{26}O$ 1504, 4.008954Diisobutyl maleate $C_{12}H_{20}O_4$ 1624, 4.4649001-Dodecanaline, N,N-dimethyl- $C_{14}H_{31}N$ 1704, 3.616942Tridecanal $C_{12}H_{26}O_2$ 2120, 4.040906	Benzamide	C ₇ H ₇ NO	968, 6.027	854
Capric acid $C_{10}H_{20}O_2$ 1016, 3.344898Benzaldehyde, 4-hydroxy- $C_7H_6O_2$ 1024, 5.384935Tropeolin C_8H_7NS 1032, 5.216864E-11,13-Tetradecadien-1-0l $C_{14}H_{26}O$ 1064, 3.0379222(3H)-Furanone, dihydro-5-pentyl- $C_9H_{16}O_2$ 1064, 4.3528741-Tetradecene $C_{12}H_{24}O$ 1208, 3.352916Dodecanal $C_{12}H_{24}O$ 1208, 3.352901Acenaphthylene $C_{12}H_8$ 1472, 6.8729251-Dodecanol $C_{12}H_{20}O_4$ 1624, 4.4649001-Dodecanamine, N,N-dimethyl- $C_{14}H_{31}N$ 1704, 3.616942Tridecanal $C_{12}H_{20}O_4$ 2120, 4.040906	Capric acid	$C_{10}H_{20}O_2$	1008, 3.184	897
Benzaldehyde, 4-hydroxy- $C_7H_6O_2$ 1024, 5.384935Tropeolin C_8H_7NS 1032, 5.216864E-11,13-Tetradecadien-1-ol $C_{14}H_{26}O$ 1064, 3.0379222(3H)-Furanone, dihydro-5-pentyl- $C_9H_{16}O_2$ 1064, 4.3528741-Tetradecene $C_{14}H_{28}$ 1128, 2.600944Dodecanal $C_{12}H_{24}O$ 1208, 3.352916Coumarin $C_9H_6O_2$ 1408, 8.263901Acenaphthylene $C_{12}H_8$ 1472, 6.8729251-Dodecanol $C_{12}H_{26}O$ 1504, 4.008954Diisobutyl maleate $C_{12}H_{20}O_4$ 1624, 4.4649001-Dodecanaline, N,N-dimethyl- $C_{13}H_{26}O$ 1744, 4.485890Lauric acid $C_{12}H_{24}O_2$ 2120, 4.040906	Capric acid	$C_{10}H_{20}O_2$	1016, 3.344	898
Tropeolin C_8H_7NS 1032, 5.216864E-11,13-Tetradecadien-1-ol $C_{14}H_{26}O$ 1064, 3.0379222(3H)-Furanone, dihydro-5-pentyl- $C_9H_{16}O_2$ 1064, 4.3528741-Tetradecene $C_{14}H_{28}$ 1128, 2.600944Dodecanal $C_{12}H_{24}O$ 1208, 3.352916Coumarin $C_9H_6O_2$ 1408, 8.263901Acenaphthylene $C_{12}H_8$ 1472, 6.8729251-Dodecanol $C_{12}H_{26}O$ 1504, 4.008954Diisobutyl maleate $C_{12}H_{20}O_4$ 1624, 4.4649001-Dodecanaline, N,N-dimethyl- $C_{14}H_{31}N$ 1704, 3.616942Tridecanal $C_{12}H_{26}O$ 1544, 4.485890Lauric acid $C_{12}H_{20}O_2$ 2120, 4.040906	Benzaldehyde, 4-hydroxy-	$C_7H_6O_2$	1024, 5.384	935
E-11,13-Tetradecadien-1-01 $C_{14}H_{26}O$ 1064, 3.0379222(3H)-Furanone, dihydro-5-pentyl- $C_9H_{16}O_2$ 1064, 4.3528741-Tetradecene $C_{14}H_{28}$ 1128, 2.600944Dodecanal $C_{12}H_{24}O$ 1208, 3.352916Coumarin $C_9H_6O_2$ 1408, 8.263901Acenaphthylene $C_{12}H_8$ 1472, 6.8729251-Dodecanol $C_{12}H_{26}O$ 1504, 4.008954Diisobutyl maleate $C_{12}H_{20}O_4$ 1624, 4.4649001-Dodecanamine, N,N-dimethyl- $C_{14}H_{31}N$ 1704, 3.616942Tridecanal $C_{12}H_{26}O$ 1744, 4.485890Lauric acid $C_{12}H_{20}O_2$ 2120, 4.040906	Tropeolin	C ₈ H ₇ NS	1032, 5.216	864
$\begin{array}{llllllllllllllllllllllllllllllllllll$	E-11,13-Tetradecadien-1-ol	C ₁₄ H ₂₆ O	1064, 3.037	922
1-Tetradecene $C_{14}H_{28}$ 1128, 2.600944Dodecanal $C_{12}H_{24}O$ 1208, 3.352916Coumarin $C_9H_6O_2$ 1408, 8.263901Acenaphthylene $C_{12}H_8$ 1472, 6.8729251-Dodecanol $C_{12}H_{26}O$ 1504, 4.008954Diisobutyl maleate $C_{12}H_{20}O_4$ 1624, 4.4649001-Dodecanamine, N,N-dimethyl- $C_{13}H_{26}O$ 1744, 4.485890Lauric acid $C_{12}H_{24}O_2$ 2120, 4.040906	2(3H)-Furanone, dihydro-5-pentyl-	$C_9H_{16}O_2$	1064, 4.352	874
Dodecanal C ₁₂ H ₂₄ O 1208, 3.352 916 Coumarin C ₉ H ₆ O ₂ 1408, 8.263 901 Acenaphthylene C ₁₂ H ₈ 1472, 6.872 925 1-Dodecanol C ₁₂ H ₂₆ O 1504, 4.008 954 Diisobutyl maleate C ₁₂ H ₂₀ O ₄ 1624, 4.464 900 1-Dodecanamine, N,N-dimethyl- C ₁₄ H ₃₁ N 1704, 3.616 942 Tridecanal C ₁₃ H ₂₆ O 1744, 4.485 890 Lauric acid C ₁₂ H ₂₄ O ₂ 2120, 4.040 906	1-Tetradecene	C ₁₄ H ₂₈	1128, 2.600	944
Coumarin $C_9H_6O_2$ 1408, 8.263901Acenaphthylene $C_{12}H_8$ 1472, 6.8729251-Dodecanol $C_{12}H_{26}O$ 1504, 4.008954Diisobutyl maleate $C_{12}H_{20}O_4$ 1624, 4.4649001-Dodecanamine, N,N-dimethyl- $C_{14}H_{31}N$ 1704, 3.616942Tridecanal $C_{12}H_{26}O$ 1744, 4.485890Lauric acid $C_{12}H_{24}O_2$ 2120, 4.040906	Dodecanal	C ₁₂ H ₂₄ O	1208, 3.352	916
Acenaphthylene C ₁₂ H ₈ 1472, 6.872 925 1-Dodecanol C ₁₂ H ₂₆ O 1504, 4.008 954 Diisobutyl maleate C ₁₂ H ₂₆ O 1624, 4.464 900 1-Dodecanamine, N,N-dimethyl- C ₁₄ H ₃₁ N 1704, 3.616 942 Tridecanal C ₁₃ H ₂₆ O 1744, 4.485 890 Lauric acid C ₁₂ H ₂₄ O ₂ 2120, 4.040 906	Coumarin	$C_9H_6O_2$	1408, 8.263	901
1-Dodecanol C ₁₂ H ₂₆ O 1504, 4.008 954 Disobutyl maleate C ₁₂ H ₂₀ O ₄ 1624, 4.464 900 1-Dodecanamine, N,N-dimethyl- C ₁₄ H ₃₁ N 1704, 3.616 942 Tridecanal C ₁₃ H ₂₆ O 1744, 4.485 890 Lauric acid C ₁₂ H ₂₄ O ₂ 2120, 4.040 906	Acenaphthylene	C ₁₂ H ₈	1472, 6.872	925
Diisobutyl maleate C ₁₂ H ₂₀ O ₄ 1624, 4.464 900 1-Dodecanamine, N,N-dimethyl- C ₁₄ H ₃₁ N 1704, 3.616 942 Tridecanal C ₁₃ H ₂₆ O 1744, 4.485 890 Lauric acid C ₁₂ H ₂₄ O ₂ 2120, 4.040 906	1-Dodecanol	$C_{12}H_{26}O$	1504, 4.008	954
1-Dodecanamine, N,N-dimethyl- C ₁₄ H ₃₁ N 1704, 3.616 942 Tridecanal C ₁₃ H ₂₆ O 1744, 4.485 890 Lauric acid C ₁₂ H ₂₄ O ₂ 2120, 4.040 906	Diisobutyl maleate	$C_{12}H_{20}O_4$	1624, 4.464	900
Tridecanal C ₁₃ H ₂₆ O 1744, 4.485 890 Lauric acid C ₁₂ H ₂₄ O ₂ 2120, 4.040 906	1-Dodecanamine, N,N-dimethyl-	$C_{14}H_{31}N$	1704, 3.616	942
Lauric acid C ₁₂ H ₂₄ O ₂ 2120, 4.040 906	Tridecanal	C ₁₃ H ₂₆ O	1744, 4.485	890
	Lauric acid	$C_{12}H_{24}O_2$	2120, 4.040	906

Name	Formula	R.T. (s)	Similarity
β-Calacorene	$C_{15}H_{20}$	2168, 3.810	807
n-Tridecan-1-ol	C ₁₃ H ₂₈ O	2184, 2.968	935
Amyl salicylate	$C_{12}H_{16}O_3$	2192, 3.600	940
Cetene	$C_{16}H_{32}$	2248, 2.240	934
2-Tetradecanone	C ₁₄ H ₂₈ O	2264, 2.512	920
Epicedrol	C ₁₅ H ₂₆ O	2304, 2.800	904
Diphenylamine	$C_{12}H_{11}N$	2344, 3.330	886
Benzophenone	C ₁₃ H ₁₀ O	2360, 3.247	937
Tributyl phosphate	$C_{12}H_{27}O_4P$	2400, 2.304	917
Cinnamaldehyde, α-pentyl-	C ₁₄ H ₁₈ O	2400, 2.520	913
8-Heptadecene	$C_{17}H_{34}$	2464, 1.950	919
n-Hexyl salicylate	$C_{13}H_{18}O_3$	2464, 2.448	929
Triaminotriazine	$C_3H_6N_6$	2472, 3.040	882
3-Phenoxy-4-fluorobenzaldehyde	$C_{13}H_9FO_2$	2472, 3.064	886
Tetradecanenitrile	$C_{14}H_{27}N$	2488, 2.288	884
4-(1,1-Dimethylheptyl)phenol	$C_{15}H_{24}O$	2512, 2.528	895
Veramoss	$C_{10}H_{12}O_4$	2520, 3.040	902
Oplopanone	$C_{15}H_{26}O_2$	2592, 2.816	803
Myristic acid	$C_{14}H_{28}O_2$	2616, 2.400	892
Benzyl Benzoate	$C_{14}H_{12}O_2$	2640, 3.360	926
Vertofix Coeur	$C_{17}H_{26}O$	2656, 2.672	856
9-Eicosene, (E)-	$C_{20}H_{40}$	2672, 2.053	903
Benzenemethanol, 3-phenoxy-	$C_{13}H_{12}O_2$	2680, 3.688	842
1H-Indole-3-carboxaldehyde	C_9H_7NO	2720, 5.016	920
Versalide	C ₁₈ H ₂₆ O	2840, 2.888	872
Methyl palmitate	$C_{17}H_{34}O_2$	2936, 2.455	795
Palmitic acid	$C_{16}H_{32}O_2$	3016, 2.848	898
Phenylethyl salicylate	$C_{15}H_{14}O_3$	3040, 3.920	854
Benzoguanamine	$C_9H_9N_5$	3176, 5.963	825
2-(2H-Benzotriazol-2-yl)-5-methylphenol	$C_{13}H_{11}N_{3}O$	3272, 4.584	845
Fluoranthene	$C_{16}H_{10}$	3272, 5.208	933
1-Octadecanol	C ₁₈ H ₃₈ O	3280, 2.808	945
Stearic acid	$C_{18}H_{36}O_2$	3464, 3.112	800
Hexadecanamide	$C_{16}H_{33}NO$	3512, 3.712	890
p-Terphenyl	$C_{18}H_{14}$	3560, 5.192	822
trans-3,5-Dimethoxystilbene	$C_{16}H_{16}O_{2}$	3656, 5.136	877

Name	Formula	R.T. (s)	Similarity
2,6-Diphenylpyridine	$C_{17}H_{13}N$	3672, 5.640	795
1,8-Diazacyclotetradecane-2,7-dione	$C_{12}H_{22}N_2O_2$	3704, 7.416	874
Tributyl acetylcitrate	C ₂₀ H ₃₄ O ₈	3712, 3.592	874
Tert-octyldiphenylamine	C ₂₀ H ₂₇ N	3776, 4.472	768
N-Methyl-N-benzyltetradecanamine	$C_{22}H_{39}N$	3864, 3.228	850
Methyl dehydroabietate	C ₂₁ H ₃₀ O ₂	3936, 4.576	864
Octadecanamide	C ₁₈ H ₃₇ NO	4016, 4.016	790
Benzo[ghi]fluoranthene	C ₁₈ H ₁₀	4072, 6.888	879
Triphenyl phosphate	C ₁₈ H ₁₅ O ₄ P	4080, 6.432	878
Diphenyl 2-ethylhexyl phosphate	C ₂₀ H ₂₇ O ₄ P	4152, 4.824	802
Isopropylphenyl diphenyl phosphate	C ₂₁ H ₂₁ O ₄ P	4432, 6.004	815
Benz[a]anthracene, 7-methyl-	$C_{19}H_{14}$	4608, 7.312	865
Tri-m-tolylphosphate	C ₂₁ H ₂₁ O ₄ P	4800, 6.536	847
Tri-p-cresyl phosphate	$C_{21}H_{21}O_4P$	4880, 6.568	761
Perylene	C ₂₀ H ₁₂	5032, 8.200	924
Squalene	C ₃₀ H ₅₀	5152, 3.480	924
Cholesta-4,6-dien-3-ol, (3β)-	C ₂₇ H ₄₄ O	5272, 4.364	861
Cholesta-3,5-diene	C ₂₇ H ₄₄	5328, 4.288	910
Piperine	C ₁₇ H ₁₉ NO ₃	5344, 8.344	921
17αH-Trisnorhopane	C ₂₇ H ₄₆	5384, 4.864	805
Benzo[b]chrysene	$C_{22}H_{14}$	5416, 7.983	790
p,p'-Dioctyldiphenylamine	C ₂₈ H ₄₃ N	5456, 4.752	909
28-Nor-17α(H)-hopane	C ₂₉ H ₅₀	5712, 4.632	900
Cholesterol	C ₂₇ H ₄₆ O	5848, 4.848	895
α-Tocopheryl acetate	C ₃₁ H ₅₂ O ₃	6040, 4.160	904
Cholesta-3,5-dien-7-one	C ₂₇ H ₄₂ O	6072, 5.394	922
Campesterol	C ₂₈ H ₄₈ O	6112, 4.872	844
Cholest-4-en-3-one	C ₂₇ H ₄₄ O	6160, 5.232	936
17α(H),21β(H)-Homohopane	C ₃₁ H ₅₄	6168, 4.648	846
Stigmasterol	C ₂₉ H ₄₈ O	6184, 4.824	808
Cholesta-4,6-dien-3-one	C ₂₇ H ₄₂ O	6224, 5.416	876
γ-Sitosterol	C ₂₉ H ₅₀ O	6320, 4.880	919
Stigmasta-3,5-dien-7-one	C ₂₉ H ₄₆ O	6528, 5.765	825
Cholesterol, 7-oxo-	C ₂₇ H ₄₄ O ₂	6568, 6.768	913

Similarity Ave. 880/1000

Pollutants



Polyaromatic Hydrocarbons





Pesticides





Phenanthrene

Pyrene





Chlorpyrifos



1st Dimension column: 30m Rxi-5ms (Non-Polar)

Polar (More ms 7sil Rxi-1 0.60m column: Dimension 2nd

Selected Pesticides

Name	Formula	R.T. (s)	Similarity	Mass Accuracy (ppm)
Chlorfenidim	$C_9H_{11}CIN_2O$	1632, 3.512	811	N/A
Diazinone	$C_{12}H_{21}N_2O_3PS$	2712, 2.872	818	-0.84
Carbaril	$C_{12}H_{11}NO_2$	2920, 4.696	818	N/A
Chlorpyrifos	$C_9H_{11}CI_3NO_3PS$	3104, 3.712	827	N/A
Thiabendazole	$C_{10}H_7N_3S$	3272, 6.424	929	0.66
trans-Chlordane	$C_{10}H_6CI_8$	3360, 4.136	788	N/A
cis-Chlorodane	$C_{10}H_6CI_8$	3440, 4.200	772	N/A
p,p'-DDE	$C_{14}H_8CI_4$	3544, 4.480	855	-0.62
Sumithrin (isomer 1)	$C_{23}H_{26}O_3$	4400, 5.184	871	-0.21
Sumithrin (isomer 2)	$C_{23}H_{26}O_{3}$	4432, 5.084	935	0.2
Permethrine	$C_{21}H_{20}CI_2O_3$	4840, 5.792	909	-0.28
Permethrine Isomer	$C_{21}H_{20}CI_2O_3$	4888, 5.816	914	-0.55
Cyfluthrin	$C_{22}H_{18}CI_2FNO_3$	5048, 5.624	751	N/A
Cyfluthrin (isomer 2)	$C_{22}H_{18}CI_2FNO_3$	5088, 5.584	805	N/A
Cyfluthrin (isomer 3)	$C_{22}H_{18}CI_2FNO_3$	5128, 5.560	817	N/A
α -Cypermethrin	$C_{22}H_{19}CI_2NO_3$	5160, 5.944	844	N/A
β-Cypermethrin	$C_{22}H_{19}CI_2NO_3$	5192, 5.936	883	N/A
Cypermethrin (isomer 3)	$C_{22}H_{19}CI_2NO_3$	5232, 5.904	869	N/A

Ave. Similarity: 845/1000



Pesticide Example 1: Complementary El & PCI



Pesticide Example 2: trans-Chlordane, El



Pesticide Example 2: trans-Chlordane, El & ECNI



Representative Halogenated Organics

Name	Formula	R.T. (s)	Similarity	PPM
Benzyl chloride	C ₇ H ₇ Cl	488, 1.952	873	0.87
Benzyl Bromide	C ₇ H ₇ Br	560, 2.263	866	0.54
3-Chlorophenyl isocyanate	C ₇ H ₄ CINO	600, 2.264	927	0.31
3-Chlorophenol	C ₆ H₅ClO	664, 2.784	896	1.32
4-Chloroaniline	C_6H_6CIN	696, 3.160	913	1.52
p-Ethylbenzylchloride	$C_9H_{11}CI$	720, 2.704	931	0.21
α-Bromomesitylene	$C_9H_{11}Br$	912, 3.528	861	-0.23
3,4-Dichlorophenyl isocyanate	C ₇ H ₃ Cl ₂ NO	944, 3.358	820	1.93
2,5-Dichloroaniline	$C_6H_5Cl_2N$	984, 7.124	933	0.59
1-Chlorododecane	$C_{12}H_{25}CI$	1504, 3.656	949	-0.8
1-Bromododecane	$C_{12}H_{25}Br$	2096, 3.768	873	N/A
2',3',4'-Trichloroacetophenone	C ₈ H ₅ Cl ₃ O	2488, 2.976	781	N/A
ТСЕР	$C_{6}H_{12}CI_{3}O_{4}P$	2632, 3.392	893	N/A
ТСРР	$C_9H_{18}CI_3O_4P$	2728, 3.064	918	N/A
Chorophene	$C_{13}H_{11}CIO$	2904, 4.120	824	1.22
TDCPP	$C_9H_{15}CI_6O_4P$	3912, 4.904	902	N/A
2,3',4'6-Tetrabromodiphenyl ether	$C_{12}H_6Br_4O$	4384, 6.528	831	0.34
2,3',4,4',5-Pentabromodiphenyl ether	$C_{12}H_5Br_5O$	5056, 7.296	892	-0.45



Ave. Similarity: 876/1000

El: Unknown FTOHs





EI & PCI: Annotated 10:2 FTOH





EI: Annotated 12:2 FTOH





Part 2 Retrospective Analysis of Data Archives



Scaled Mass Defect Plots



	FI	
0.0	0.0 -	CI-H defect = CI-H mass - nominal mass
		CI-H mass = IUPAC mass x (34/33.96102)
-0.2	-0.2-	Taguchi, et al, <i>J. Am. Mass Spectrom</i> , 2010 , <i>21</i> , 1918-1921.
Pefect (Cl-H)	-0.4- U U U U U U U U	
Scaled Mass [9.0-	Scaled Mass No.6-	
-0.8	-0.8 -	
-1.0	-1.0-	
	-0 200 400 600 800 Nominal Mass (m/z) • PCBs • Chordanes • FtOHs	

Spectral Analysis Tools



SMD (CI-H): PCBs & Chlordanes



PCBs: SMD (CI-H) to Contour Plot



🕐 🖻 🔜 🔜 🔵 🔻 Auto Select Æ Enable Target Analyte Finding TOF Enable E-TAF: Merge HRD® peak data with matching Target Analyte peaks Correction Smooth window size (points): Auto Peak FWHH (seconds): Integration Baseline: Auto-Calculated Mass Calibration Expected Adducts: A Adduct Charge Mass Delta (Da) Add.... 1* M -1 0.00055 Peak Remove Finding Target Analyte Finding List: POPs Target Analyte GCxGC Finding Analytes to Find: Analyte Form Most Tolerance Units Start Time End Time Start 2nd Dim Time Advanced . C6Cl6 3.00 PPM 2530 s 2544 s 2.784 s 2* CN CI4 3.00 PPM 2840 s 2856 s 3.208 s Add Classificati 3 CN CI4:2 3.00 PPM 2914 s 2928 s 3.447 s 4 Chlordane Isomer 1 3.00 PPM 3200 s 3216 s 3.427 s Remove P 3.984 s Heptachlor 3.00 PPM 3232 s 3239 s CB 4Cl 3.00 PPM 3264 s 3280 s 4.048 s Import ... Heptachlor 2 3.00 PPM 3328 s 3344 s 4.216 s Spectral trans-Chlordane 3.00 PPM 3352 s 3368 s 3.968 s Analysis Export... CB 4CI:2 3.00 PPM 3366 s 3370 s 4.408 s Chlordane Isomer 2 3384 s 10 3 00 PPM 3400 s 3.960 s Library... 11 CB 5CI 3.00 PPM 3392 s 3408 5 4 088 5 12 cis-Chlordane 3.00 PPM 3432 s 3448 \$ 4.040 s Shift RTs... Retention 13 3.760 s Nonachlo 3.00 PPM 3456 s 3472 s Index CB 5CI:2 14 3.00 PPM 3568 s 3584 5 4.544 s 15 CB 6Cl 3.00 PPM 3639 s 3645 s 4.304 s 16 CB 6CI:2 3.00 PPM 3647 s 3650 s 4.515 s 17 CB 5CI:3 3.00 PPM 3707 s 3720 s 4.560 s 18 Nonachlor Isomer 3 3.00 PPM 3776 s 3789 s 4.512 s Quantitate 19 CB 6CI:3 3.00 PPM 3792 s 3808 s 4.432 s Reference 20 CB 6CI:4 3.00 PPM 3824 s 3840 s 4.488 s 21 CB 6CI:5 3.00 PPM 3896 s 3912 s 4.704 s ••• 22 CB 6Cl:6 3.00 PPM 3978 s 3992 s 4.864 s 23 CB 7Cl 3.00 PPM 4072 s 4088 s 4.696 s ... 24 CB 7CI:2 3.00 PPM 4096 s 4112 s 4.808 s Annotate 25 CB 6CI:7 3.00 PPM 4128 s 4144 s 5.448 s Spectral ... 26 CB 6CI:8 3.00 PPM 4136 s 4152 s 4.800 s Data 27 CB 7CI:3 3.00 PPM 4200 s 4216 s 5.144 s ... 28 CB 7CI:4 4248 s 3.00 PPM 4232 s 5.200 s 29 CB 6CI:9 4280 s 3.00 PPM 4266 s 5.216 s CB 7CI:5 30 4320 s 4336 s 4.944 s 3.00 PPM Library 31 CB 7CI:6 4360 s 4376 s 3.00 PPM 5.032 s Search 32 CB 7CI:7 4528 s 3.00 PPM 4544 s 5.536 s 33 CB 8CI 4576 s 4592 s Options 3.00 PPM 5.144 s CB 9Cl 34 4792 s 3.00 PPM 4776 s 5.226 s 35 CB 8CI:2 3.00 PPM 4784 s 4800 s 5.680 s 36 CB 8CI:3 3.00 PPM 4904 s 4920 s 5.496 s 37 BDE-71 3.00 PPM 5048 s 5061 s 7.040 s Data CB 9CI:2 38 3.00 PPM 5120 s 5136 s 5.528 s

3.00 PPM

3.00 PPM

5304 s

3426 s

5320 s

3440 s

5.619 s

3.720 s

Export

Options

-

39

40

<

CB-209

Nonachlor Isomer 1

Targeting POPs in ECNI

✓ Trace Analysis ✓ Quantitative Analysis ✓ Fast Processing

Targeting Trace POPs in ECNI 💽 💽 🔜 🔜 🔵 👘 Auto Select Æ Enable Target Analyte Finding TOF Enable E-TAF: Merge HRD® peak data with matching Target Analyte peaks **HRAM** lons Correction Smooth window size (points): Auto Æ Input Masses For Target Analyte Finding Peak FWHH (seconds): Integration Baseline: Auto-Calculated Mass Analyte: trans-Chlordane Calibration Expected Adducts: Formula Isotope M/Z Tolerance Units Required 409.79192 R C10H6Cl8 3.00 PPM Adduct Charge Mass Delta (Da) Add Add... 1-2 407.79484 3.00 PPM 1* M -1 0.00055 1-3 411.78900 3.00 PPM Add Isotope 405.79777 PPM Peak 3.00 1-4 Remove Finding Remove Target Analyte Finding List: POPs Target Analyte GCxGC Finding Analytes to Find: * 409.79215 Analyte Form Most Tolerance Units Start Time End Time Start 2nd Dim Time 409.79215 Advanced . C6Cl6 2544 s 3.00 PPM 2530 s 2.784 2* CN CI4 3.00 PPM 2840 s 2856 s 3.208 Add Classificati. 3e4 ***** 407.79515 3 CN CI4:2 3.00 PPM 2914 s 2928 s 3.447 .78922 4 Chlordane Isomer 1 3.00 PPM 3200 s 3216 s 3.427 P Remove -0.05 PPM 3232 s 3239 s 3.984 Heptachlor 3.00 PPM 3280 s 4.048 CB 4Cl 3.00 PPM 3264 s Import ... 4.216 s 411. Heptachlor 2 3.00 PPM 3328 s 3344 s Spectral M⁻• trans-Chlordane 3.00 PPM 3352 s 3368 s 3.968 s Analysis Export... CR 4CF 3366.5 3370 5 4.408 9 3.00 PPI 4 10 Chlordane Isomer 2 3384 s 3400 s 3.960 s 3.00 PPM Library... 79824 11 CB 5Cl 3408 s 4.088 s 3.00 PPM 3392 s cis-Chlordane 12 3.00 PPM 3432 s 3448 s 4.040 s 78655 Shift RTs... Retention 13 Nonachlor 3.760 s 3.00 PPM 3456 s 3472 s 373.8342 405. 2e4 Index 14 CB 5CI:2 3568 s 4.544 s trans-Chlordane 3.00 PPM 3584 s 15 CB 6Cl 3.00 PPM 3639 s 3645 s 4.304 s ΓD 16 CB 6CI:2 3.00 PPM 3647 s 3650 s 4.515 s (m 17 CB 5CI:3 3.00 PPM 3707 s 3720 s 4.560 s \sim 18 Nonachlor Isomer 3 3.00 PPM 3776 s 3789 s 4.512 s Quantitate 9043. 19 CB 6CI:3 3.00 PPM 3792 s 3808 s 4.432 s Reference 20 CB 6CI:4 3.00 PPM 3824 s 3840 s 4.488 s 21 CB 6CI:5 3.00 PPM 3896 s 3912 s 4.704 s ••• 22 CB 6CI:6 3.00 PPM 3978 s 3992 s 4.864 s 23 CB 7Cl 3.00 PPM 4072 s 4088 s 4.696 s <u>ں</u> ••• 24 CB 7CI:2 3.00 PPM 4096 s 4112 s 4.808 s 26 Annotate 25 CB 6CI:7 3.00 PPM 4128 s 4144 s 5.448 s Spectral 1e4 ... 26 CB 6CI:8 3.00 PPM 4136 s 4152 s 4.800 s 405 410 415 Data 27 CB 7CI:3 3.00 PPM 4200 s 4216 s 5.144 s ... 28 CB 7CI:4 3.00 PPM 4232 s 4248 s 5.200 s C 29 CB 6CI:9 4266 s 4280 s 3.00 PPM 5.216 s ••• CB 7CI:5 4336 s 30 3.00 PPM 4320 s 4.944 s Library 31 CB 7CI:6 3.00 PPM 4360 s 4376 5 5.032 s Search 32 CB 7CI:7 4528 s 4544 s 3.00 PPM 5.536 s 33 CB 8Cl 4592 s 3.00 PPM 4576 s 5.144 s Options CB 9Cl 34 4776 s 4792 s 3.00 PPM 5.226 s 35 CB 8CI:2 4784 s 4800 s 3.00 PPM 5.680 s 36 CB 8CI:3 4920 s 3.00 PPM 4904 s 5.496 s 0 37 BDE-71 3.00 PPM 5048 s 5061 s 7.040 s Data 38 CB 9CI:2 3.00 PPM 5120 s 5136 s 5.528 s M/Z 200 300 400 500 600 Export 39 CB-209 3.00 PPM 5304 s 5320 s 5.619 s Options 40 Nonachlor Isomer 1 3.00 PPM 3426 s 3440 s 3.720 s < > -

TAF Results: Trace POPs in NIST SRM



TAF Results: NIST SRM, Household, and Office Dust

Target POP	R.T. (s)	NIST (area)	Office (area)	House (area)	Target POP	R.T. (s)	NIST (area)	Office (area)	House (area
C ₆ Cl ₆	2536, 2.872	66777	10364	485688	CB 6CI:4	3832, 4.640	285099	324443	
CN Cl4	2848, 3.304	13710			CB 6CI:5	3904, 4.872	85405	83716	
CN Cl4:2	2920, 3.568	143301			CB 6CI:6	3984, 5.096	280450	328292	
Chlordane Isomer 1	3208, 3.552	62129			CB 7Cl	4080, 4.864	149348	108803	
Heptachlor 1	3232, 4.128	15887			CB 7CI:2	4104, 4.952	68723	50837	
CB 4Cl	3272, 4.192	21645	8827		CB 6CI:7	4136, 5.632	39203	47433	
Heptachlor 2	3336, 4.360	215913			CB 6CI:8	4144, 4.976	27026	22346	
trans-Chlordane	3360, 4.112	1730979	3025	11470	CB 7CI:3	4208, 5.304	92038	91365	
CB 4CI:2	3368, 4.552	10321	1454		CB 7CI:4	4240, 5.376	38110	38962	
Chlordane Isomer 2	3392, 4.096	266412			CB 6CI:9	4272, 5.392	67431	66771	
CB 5Cl	3400, 4.224	54160	50338		CB 7CI:5	4328, 5.120	26105	19932	
Nonachlor Isomer 1	3432, 3.848	9577			CB 7CI:6	4368, 5.200	397534	369028	
cis-Chlordane	3440, 4.176	624489			CB 7CI:7	4536, 5.720	86694	109695	
Nonachlor	3464, 3.888	596640		3023	CB 8Cl	4584, 5.312	119235	53370	
CB 5CI:2	3584, 4.720	44766	55571		CB 9Cl	4784, 5.416	13906		
CB 6Cl	3640, 4.536	23649	33324		CB 8CI:2	4792, 5.864	27430	15635	
CB 6CI:2	3648, 4.520	23937			CB 8CI:3	4912, 5.672	94752	58564	
CB 5CI:3	3712, 4.712	304119	305058		BDE-71	5056, 7.288	5480469	433778	663837
Nonachlor Isomer 3	3784, 4.656	98500			CB 9CI:2	5128, 5.720	51490	10114	
CB 6CI:3	3800, 4.576	44400	46349		CB-209	5312, 5, 792	9879		

Results: NIST SRM, Household, and Office Dust

Target POP	R.T. (s)	NIST (area)	Office (area)	House (area)	Target POP	R.T. (s)	NIST (area)	Office (area)	House
C ₆ Cl ₆	2536, 2.872	66777	10364	485688	CB 6CI:4	3832, 4.640	285099	324443	
CN Cl4	2848, 3.304	13710			CB 6CI:5	3904, 4.872	85405	83716	
CN Cl4:2	2920, 3.568	143301			CB 6CI:6	3984, 5.096	280450	328292	
Chlordane Isomer 1	3208, 3.552	62129			CB 7Cl	4080, 4.864	149348	108803	
Heptachlor 1	3232, 4.128	15887			CB 7CI:2	4104, 4.952	68723	50837	
CB 4Cl	3272, 4.192	21645	8827		CB 6CI:7	4136, 5.632	39203	47433	
Her act or	33: 1, 4 260	215913	IC	T /		4144 4 976	2 [°])26	22346	
tra s-cnlo dane	3360, 4. 12	173097	3025	114-	<u> 2</u> F 7C 3	420 ,504	950 5	9 36	54
CB 4CI:2	3368, 4.552	10321	1454		Св 7СІ:4	4240, 5.376	38110	3896Z	
Chlordane Isomer 2	3392, 4.096	266412			CB 6Cl.9	4272, 5.392	67431	66771	
CB 5Cl	3400, 4.224	54160	50338		CB 7CI:5	4328, 5.120	26105	19932	
Nonachlor Isomer 1	3432, 3.848	9577			CB 7CI:6	4368, 5.200	397534	369028	
cis-Chlordane	3440, 4.176	624489			CB 7CI:7	4536, 5.720	86694	109695	
Nonachlor	3464, 3.888	596640		3023	CB 8Cl	4584, 5.312	119235	53370	
CB 5CI:2	3584, 4.720	44766	55571		CB 9Cl	4784, 5.416	13906		
CB 6Cl	3640, 4.536	23649	33324		CB 8CI:2	4792, 5.864	27430	15635	
CB 6CI:2	3648, 4.520	23937			CB 8CI:3	4912, 5.672	94752	58564	
CB 5CI:3	3712, 4.712	304119	305058		BDE-71	5056, 7.288	5480469	433778	66
Nonachlor Isomer 3	3784, 4.656	98500			CB 9CI:2	5128, 5.720	51490	10114	
CB 6CI:3	3800, 4.576	44400	46349		CB-209	5312, 5.792	9879		

Part 3

Quantitative Analysis of Polychlorinated Paraffins

Short Chain (SCCPs): C_{10} to C_{13} Medium Chain (MCCPs): C_{14} to C_{17}







Standard Mix :

SCCP 51.5%, 55.5%, 63%; MCCP 42%, 52%, 57%

- CS1 0.25 ppm
- CS2 0.50 ppm
- CS3 1.0 ppm
- CS4 3.0 ppm
- CS5 5.0 ppm
- CS6 7.0 ppm
- CS7 10.0 ppm*
- CS8 15.0 ppm



Std. Mix: Contour Plot & Mass Spectra for G4 Region



Cloud Quant Data Processing

Method: Mass Calibration, Signal Processing & Classification

A	uto Select		🖻 🔒 🔣 🔓	\$ +	1 🖪 🗑 🖉 🖾) =													
#	Show	Class	Comp Region	Color	Formula 1	Data I	Mass Toleran	Formula 2	Data	Mass Toleran	Formula 3	Data I	Mass Toleran	Formula 4	Data D	d Mass Tolera	n Formula 5	Data I	Mass Tolera	n Formula 6
1		<u>G1</u>	.	0	277.9982 279.9952	Signal	5 PPM		Signal			Signal			Signal			Signal		
2		<u>G2</u>			312.9671 314.9664	Signal	5 PPM	292.0132 294.0199	Signal	5 PPM		Signal			Signal			Signal		
3		<u>G3</u>	E	0	346.9285 348.9257	Signal	5 PPM	325.9752 327.9730	Signal	5 PPM	304.0340 306.0301	Signal	5 PPM		Signal			Signal		
4		<u>G4</u>	E	0	360.9438 362.9407	Signal	5 PPM	339.9909 341.9888	Signal	5 PPM		Signal			Signal			Signal		
5		<u>G5</u>	E		380.8888 382.8862	Signal	5 PPM	394.9048 396.9006	Signal	5 PPM	374.9594 376.9556	Signal	5 PPM	354.0056 356.0036	Signal	5 PPM		Signal		
6		<u>G6</u>	E	0	430.8621 432.8593	Signal	5 PPM	408.9207 410.9168	Signal	5 PPM	388.9745 390.9722	Signal	5 PPM	368.0223 370.0195	Signal	5 PPM		Signal		
7		<u>G7</u>			464.8241 466.8210	Signal	5 PPM	444.8788 446.8760	Signal	5 PPM	422.9361 424.9334	Signal	5 PPM	402.9906 404.9877	Signal	5 PPM	382.0370 384.0349	Signal	5 PPM	366.0053 368.0022
8		<u>G8</u>			478.8385 480.8350	Signal	5 PPM	458.8927 460.8896	Signal	5 PPM	436.9519 438.9486	Signal	5 PPM	417.0063 419.0030	Signal	5 PPM	396.0527 398.0511	Signal	5 PPM	
9		<u>G9</u>			492.8536 494.8505	Signal	5 PPM	472.9098 474.9066	Signal	5 PPM	450.9686 452.9657	Signal	5 PPM	431.0151 433.0197	Signal	5 PPM	411.0767 413.0739	Signal	5 PPM	
10		<u>G10</u>	.		506.8710 508.8684	Signal	5 PPM	486.9258 488.9231	Signal	5 PPM	464.9828 466.9802	Signal	5 PPM	445.0368 447.0342	Signal	5 PPM		Signal		
11		<u>G11</u>	.		520.8865 522.8838	Signal	5 PPM	500.9415 502.9389	Signal	5 PPM	480.9955 482.9932	Signal	5 PPM		Signal			Signal		
12		<u>G12</u>	E		534.9021 536.9006	Signal	5 PPM	514.9581 516.9546	Signal	5 PPM		Signal			Signal			Signal		
13*		ISTD	E		260.9087 262.90577	Signal	5 PPM		Signal			Signal			Signal			Signal		
14		Unclass				Signal	5 PPM		Signal	5 PPM		Signal			Signal			Signal		

- SCCP & MCCP formula congeners analyzed simultaneously in one injection
- Analysis restricted to SCCP/MCCP congeners with 10-17 Carbon & 5-10 Chlorine atoms
- CP formula congener group quantification of cloud group patterns (Classification) with HRAM Formulas
- Utilized the most abundant m/z values in the [M-CI]⁻ or [M-HCI]⁻ isotope clusters

Cloud Quant Data Processing

Method: Mass Calibration, Signal Processing & Classification

- A	uto Select			18 +	白鴨 油 🖌 🖽	/二 🎑) 🔻										
#	Show	Class	Comp Region	Color	Formula 1	Data I Mass Tolerar	Formula 2	Data Mass To	oleran Formula 3	Data Mass Tole	eran Formula 4	Data D	C Mass Tole	an Formula 5	Data Mass Tole	eran Formula 6
1		<u>G1</u>	. E		277.9982 279.9952	Signal 5 PPM		Signal		Signal		Signal			Signal	
2		<u>G2</u>			312.9671 314.9664	Signal 5 PPM	292.0132 294.0199	Signal 5 PPM		Signal		Signal			Signal	
3		<u>G3</u>		\odot	346.9285 348.9257	Signal 5 PPM	325.9752 327.9730	Signal 5 PPM	304.0340 306.0301	Signal 5 PPM		Signal			Signal	
4		<u>G4</u>	.		360.9438 362.9407	Signal 5 PPM	339.9909 341.9888	Signal 5 PPM		Signal		Signal			Signal	
5		<u>G5</u>	.		380.8888 382.8862	Signal 5 PPM	394.9048 396.9006	Signal 5 PPM	374.9594 376.9556	Signal 5 PPM	354.0056 356.0036	Signal	5 PPM		Signal	
6	\square	<u>G6</u>			430.8621 432.8593	Signal 5 PPM	408.9207 410.9168	Signal 5 PPM	388.9745 390.9722	Signal 5 PPM	368.0223 370.0195	Signal	5 PPM		Signal	
7		<u>G7</u>			464.8241 466.8210	Signal 5 PPM	444.8788 446.8760	Signal 5 PPM	422.9361 424.9334	Signal 5 PPM	402.9906 404.9877	Signal	5 PPM	382.0370 384.0349	Signal 5 PPM	366.0053 368.0022
8		<u>G8</u>	E		478.8385 480.8350	Signal 5 PPM	458.8927 460.8896	Signal 5 PPM	436.9519 438.9486	Signal 5 PPM	417.0063 419.0030	Signal	5 PPM	396.0527 398.0511	Signal 5 PPM	
9		<u>G9</u>	.	\odot	492.8536 494.8505	Signal 5 PPM	472.9098 474.9066	Signal 5 PPM	450.9686 452.9657	Signal 5 PPM	431.0151 433.0197	Signal	5 PPM	411.0767 413.0739	Signal 5 PPM	
10		<u>G10</u>			506.8710 508.8684	Signal 5 PPM	486.9258 488.9231	Signal 5 PPM	464.9828 466.9802	Signal 5 PPM	445.0368 447.0342	Signal	5 PPM		Signal	
11		<u>G11</u>			520.8865 522.8838	Signal 5 PPM	500.9415 502.9389	Signal 5 PPM	480.9955 482.9932	Signal 5 PPM		Signal			Signal	
12		<u>G12</u>	E		534.9021 536.9006	Signal 5 PPM	514.9581 516.9546	Signal 5 PPM		Signal		Signal			Signal	
13*		ISTD	.		260.9087 262.90577	7 Signal 5 PPM		Signal		Signal		Signal			Signal	
14		Unclas	8			Signal 5 PPM		Signal 5 PPM		Signal		Signal			Signal	

Results: Mass Calibration (PFTBA)

lon	Formula	m/z calc	m/z obs	PPM
PFTBA200	C_4F_8	199.9878	199.9878	0.11
PFTBA283	$C_5F_{11}N$	282.9861	282.9860	-0.15
PFTBA395	$C_8F_{15}N$	394.9797	394.9796	-0.28
PFTBA414	$C_8F_{16}N$	413.9781	413.9780	-0.27
PFTBA433	$C_8F_{17}N$	432.9765	432.9765	0.04
PFTBA452	$C_8F_{18}N$	451.9749	451.9749	0.03
PFTBA514	$C_{10}F_{20}N$	513.9717	513.9716	-0.24
PFTBA595	$C_{12}F_{23}N$	594.9669	594.9668	-0.14
PFTBA633	$C_{12}F_{25}N$	632.9637	632.9637	0.03

Signal Processing/Classification

#	Class	Formula 1	Formula 2	Formula 3	Formula 4	Formula 5
1*	G1	5647020.8				
2	G2	5337271.5	656267.5			••••••••••••••••••••••••••••••••••••••
3	G3	5255488.5	44026336.7	4689636.2		
4	G4	79009169.5	37677291.8			
5	G5	6728968.5	36301486.7	41784563.4	13809033.1	
6	G6	4339475.0	38949714.0	17461083.8	27230197.5	
7	G7	2067782.9	23885494.7	21835898.0	30198738.6	4551473.4
8	G8	344645.8	120905.5	36278044.2	4257813.1	237496.1
9	G9	49485.0	8679982.3	140282.9	61940.5	49.1
10	G10	869019.4	2087095.8	483837.0	5876.8	
11	G11	211600.2	181369.9	8775.4		
12	G12	9366.9	5732.6			
13	ISTD	1179072.9				
	Total	95176852.4	.54544763.9	82847158.6	44695910.7	4615599.4

Cloud Quant Results: NIST SRM, Group 4

NIST SRM



Cloud Quant Results: NIST SRM, SCCP & MCCP

NIST SRM

		Group	PCP (µg/mL)
	SCCP _{tot}	G1	0.66
	11.1.4.4	G2	0.61
	11.1 µg/g	G3	0.31
	C_{10} - C_{13}	G4	0.48
		G5	0.74
	MCCP _{tot}	G6	0.58
		G7	0.95
	11.2 μg/g	G8	0.86
	C = C	G9	0.59
	014-017	G10	0.85
1000	2000	3000	4000

Cloud Quant Results: NIST SRM, SCCP & MCCP

NIST SRM

		Group	PCP (μg/mL)
	SCCP _{tot}	G1	0.66
	11.1.4.4	G2	0.61
	11.1 µg/g	G3	0.31
	C_{10} - C_{13}	G4	0.48
		G5	0.74
	MCCP _{tot}	G6	0.58
		G7	0.95
	11.2 μg/g	G8	0.86
	C - C	G9	0.59
	014-017	G10	0.85
1000	2000	3000	4000

	Ref. 1	Ref. 2	Ref. 3
SCCP (µg/g)	7.6	8.7	7.1
MCCP (µg/g	16.4	12.0	10.0

- 1) Shang, et al, *Environ. Sci. Pollut. Res.* **2019**, *26*, 7453-7462.
- 2) Brits, et al, *Chemosphere* **2020**, *238*, 124643.
- 3) Brandsma, et al, *Environ. Sci. Technol.* **2019**, *53*, 7595-7604.

Cloud Quant Results: NIST SRM & Household Dust

PCP (µg/mL) Group ECNI (XIC) SCCP_{tot} G1 0.66 G2 0.61 11.1 μg/g G3 0.31 C_{10} - C_{13} 0.48 G4 G5 0.74 MCCP_{tot} G6 0.58 G7 0.95 11.2 μg/g **G8** 0.86 **G9** 0.59 C_{14} - C_{17} 0.85 G10 4000 1000 2000 3000

NIST SRM



Household

Summary





- GCxGC-HRTOFMS is a powerful discovery tool
 - MMS El mode: Compound characterization samples
 - ✓ Database comparisons
 - ✓ Formula determinations (HRAM ions)
 - Complementary Ionization modes for compound annotation
 - Retrospective Analysis using software tools (e.g., scaled mass defect plots)

Summary



- GCxGC-HRTOFMS is a powerful discovery tool
 - MMS El mode: Compound characterization samples
 - ✓ Database comparisons
 - ✓ Formula determinations (HRAM ions)
 - Complementary Ionization modes for compound annotation
 - Retrospective Analysis using software tools (e.g., scaled mass defect plots)
- Effective Dust PCP Cloud Quant Analysis
 - Mass calibration (HRAM ions)
 - Group classification + signal processing





Thank you very much for your attention.