**EXTRACT MeOH WITH FILTER PVDF**

Data File : 191129004.D

Acq On : 29 Nov 2019 13:22 (#1); 29 Nov 2019 13:17 (#2)

Operator: KAREN MENDEZ

Sample : EXTRACTO METOH PDVF

Search Libraries: C:\Database\NIST98.L Minimum Quality: 0

Pk# RT Area% Library/ID Ref# CAS# Qual

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

1 8.217 1.17 C:\Database\NIST98.L

Dodecane, 2,6,11-trimethyl- 112569 031295-56-4 64

Octane, 2,3,6,7-tetramethyl- 6367 052670-34-5 64

Octane, 2,3,6-trimethyl- 17068 062016-33-5 59

2 8.331 1.78 C:\Database\NIST98.L

Decane, 2,3,5,8-tetramethyl- 16393 1000149-58-9 64

Heptane, 3,3,5-trimethyl- 114596 007154-80-5 64

Octane, 2,3,6,7-tetramethyl- 6367 052670-34-5 64

3 10.271 1.59 C:\Database\NIST98.L

2-Undecene, 4-methyl- 22861 1000061-82-8 46

Heptane, 4-methylene- 22748 015918-08-8 43

2-Heptene, 4-methyl-, (E)- 22241 066225-17-0 38

4 10.397 2.24 C:\Database\NIST98.L

2-Undecene, 4-methyl- 22861 1000061-82-8 46

Cyclooctane, 1-methyl-3-propyl- 23096 1000151-39-4 43

Heptane, 4-methylene- 22748 015918-08-8 38

5 15.352 4.19 C:\Database\NIST98.L

Benzene, 1,3-bis(1,1-dimethylethyl 125073 001014-60-4 95

)-

Benzene, 1,3-bis(1,1-dimethylethyl 125075 001014-60-4 87

)-

Benzene, 1,4-bis(1,1-dimethylethyl 125076 001012-72-2 86

)-

6 16.748 2.78 C:\Database\NIST98.L

R-(+)-Methyl-2-isopropyl-5-oxohexa 6135 1000108-54-7 53

noate

Cyclooctane, 1-methyl-3-propyl- 23096 1000151-39-4 35

Cyclooctane, butyl- 23309 016538-93-5 35

7 16.977 2.95 C:\Database\NIST98.L

R-(+)-Methyl-2-isopropyl-5-oxohexa 6135 1000108-54-7 49

noate

Cyclohexane, 1,1-dimethyl-2-propyl 22875 081983-71-3 46

Cyclohexane, 1,3,5-trimethyl- 22841 001839-63-0 35

8 17.206 2.19 C:\Database\NIST98.L

4-Isopropyl-1,3-cyclohexanedione 22410 062831-62-3 60

Cyclohexane, 1,2,4-trimethyl- 114309 002234-75-5 35

Heptane, 4-methylene- 22748 015918-08-8 35

9 17.280 1.03 C:\Database\NIST98.L

Tridecane, 1-iodo- 16508 035599-77-0 86

Heptadecane 112319 000629-78-7 59

Dodecane, 2,6,11-trimethyl- 109635 031295-56-4 58

10 21.252 1.00 C:\Database\NIST98.L

Hexadecane, 7-methyl- 17103 026730-20-1 72

Undecane, 5-ethyl-5-propyl- 16408 002755-07-9 53

Decane, 5-ethyl-5-methyl- 17108 017312-74-2 53

11 22.058 2.21 C:\Database\NIST98.L

Phenol, 2,4-bis(1,1-dimethylethyl) 125781 000096-76-4 94

Phenol, 2,4-bis(1,1-dimethylethyl) 125783 000096-76-4 93

Phenol, 2,4-bis(1,1-dimethylethyl) 125776 000096-76-4 93

12 22.304 1.31 C:\Database\NIST98.L

6-Tridecene, 7-methyl- 111541 024949-42-6 49

3-Hexene, 2,2,5,5-tetramethyl-, (Z 2647 000692-47-7 41

)-

Cyclohexane, 1,2,4-trimethyl- 22847 002234-75-5 41

13 22.533 1.08 C:\Database\NIST98.L

Bacchotricuneatin c 24581 066563-30-2 43

Cyclohexane, 1,1,3,5-tetramethyl-, 114330 050876-32-9 30

cis-

2-Heptene, 4-methyl-, (E)- 22241 066225-17-0 25

14 22.699 1.80 C:\Database\NIST98.L

Decane, 2,3,6-trimethyl- 5623 062238-12-4 64

Tridecane, 1-iodo- 16508 035599-77-0 64

Triacontane 17141 000638-68-6 64

15 22.957 1.66 C:\Database\NIST98.L

Cyclopentane, (2-methylbutyl)- 22257 053366-38-4 38

3-Hexene, 2,2,5,5-tetramethyl-, (Z 2647 000692-47-7 38

)-

Bacchotricuneatin c 24581 066563-30-2 30

16 27.374 1.25 C:\Database\NIST98.L

Cyclohexane, 1-ethyl-2-propyl- 22848 062238-33-9 43

3-Hexene, 2,2,5,5-tetramethyl-, (Z 2647 000692-47-7 30

)-

10-Methylnonadecane 17087 056862-62-5 27

17 27.792 1.58 C:\Database\NIST98.L

3-Hexene, 2,2,5,5-tetramethyl-, (Z 2647 000692-47-7 38

)-

Cyclohexane, 1,1,3,5-tetramethyl-, 114329 050876-31-8 30

trans-

Cyclohexane, 1,1,3,5-tetramethyl-, 114330 050876-32-9 25

cis-

18 27.975 1.19 C:\Database\NIST98.L

Bacchotricuneatin c 24581 066563-30-2 27

Cyclohexane, 1,1,3,5-tetramethyl-, 114330 050876-32-9 25

cis-

3-Hexene, 2,2,5,5-tetramethyl-, (Z 2647 000692-47-7 25

)-

19 28.244 0.99 C:\Database\NIST98.L

Cyclohexane, 1-ethyl-2-propyl- 22848 062238-33-9 38

Cyclohexane, 1,2-diethyl-3-methyl- 22852 061141-80-8 30

Heptane, 4-methylene- 22748 015918-08-8 30

20 28.490 1.06 C:\Database\NIST98.L

Cyclohexane, 1,2,4-trimethyl- 22847 002234-75-5 45

Cyclohexane, 1,2-diethyl-3-methyl- 22852 061141-80-8 30

Cyclohexane, 1-ethyl-2,4-dimethyl- 23318 061142-69-6 27

21 31.751 4.67 C:\Database\NIST98.L

n-Hexadecanoic acid 114901 000057-10-3 97

n-Hexadecanoic acid 6589 000057-10-3 86

Tridecanoic acid 114895 000638-53-9 70

22 35.425 2.14 C:\Database\NIST98.L

Octadecanoic acid 114902 000057-11-4 93

Octadecanoic acid 6590 000057-11-4 74

Octadecanoic acid 109378 000057-11-4 68

23 36.792 1.00 C:\Database\NIST98.L

3-Decene, 2,2-dimethyl-, (E)- 23098 055499-02-0 46

Cyclohexane, 1,2,4-trimethyl- 114210 002234-75-5 38

Docosane 16531 000629-97-0 30

24 46.428 1.14 C:\Database\NIST98.L

Octadecanoic acid, 2-(acetyloxy)-1 9075 055401-62-2 68

-[(acetyloxy)methyl]ethyl ester

Eicosanoic acid, 2,3-bis(acetyloxy 9074 055429-67-9 40

)propyl ester

Eicosanoic acid, 2-(acetyloxy)-1-[ 9077 055429-68-0 38

(acetyloxy)methyl]ethyl ester

25 46.525 3.49 C:\Database\NIST98.L

Octadecanoic acid, 2-(acetyloxy)-1 9075 055401-62-2 62

-[(acetyloxy)methyl]ethyl ester

Hexadecanoic acid, 2,3-bis(acetylo 70191 055268-70-7 43

xy)propyl ester

Eicosanoic acid, 2,3-bis(acetyloxy 9074 055429-67-9 42

)propyl ester

26 46.726 1.41 C:\Database\NIST98.L

Tetrapentacontane, 1,54-dibromo- 17122 1000156-09-4 76

Acetic acid, octadecyl ester 109492 000822-23-1 64

17-Pentatriacontene 5525 006971-40-0 58

27 49.690 11.33 C:\Database\NIST98.L

di-n-Nonyl sulfide 70212 000929-98-6 16

Benzene, trichloro[(dichlorophenyl 70396 074421-51-5 12

)methoxy]-

1,3-Dioxane-5-carboxylic acid, 2-( 70240 119620-07-4 12

1,1-dimethylethyl)-4,6-dimethyl-,

(2.alpha.,4.alpha.,5.beta.,6.alpha

.)-

28 49.793 33.07 C:\Database\NIST98.L

Phosphonic acid, phenyl-, bis[5-me 70203 061048-72-4 37

thyl-2-(1-methylethyl)cyclohexyl]

ester

Oxazole, 5-methyl-2-phenyl- 124089 005221-67-0 32

3-Benzyl-1H-1,2,4-triazole 70350 021117-34-0 23

29 52.225 1.78 C:\Database\NIST98.L

4-Dehydroxy-N-(4,5-methylenedioxy- 84754 1000111-66-9 37

2-nitrobenzylidene)tyramine

Tetrasiloxane, decamethyl- 126458 000141-62-8 35

Acetamide, N-[4-(trimethylsilyl)ph 126472 017983-71-0 30

enyl]-

30 53.907 4.90 C:\Database\NIST98.L

9-O-Pivaloyl-N-acetylcolchinol 106352 1000127-10-7 50

4-Benzoyl-N-(4-methylbenzylidene)- 106349 095855-26-8 42

3,5-diphenyl-2-furanamine

N-Acetoacetyl-deacetylcolchicine 10095 1000127-13-2 9

**EXTRACT MeOH WITH FILTER PTFE**

Data File : 191129005.D

Acq On : 29 Nov 2019 14:24 (#1); 29 Nov 2019 14:19 (#2)

Operator : KAREN MENDEZ

Sample : EXTRACTO METOH PTFE

Search Libraries: C:\Database\NIST98.L Minimum Quality:

Pk# RT Area% Library/ID Ref# CAS# Qual

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1 8.331 1.44 C:\Database\NIST98.L

Heptane, 3,3,5-trimethyl- 114594 007154-80-5 64

Decane, 4-methyl- 109903 002847-72-5 64

Octane, 2,3,6,7-tetramethyl- 6367 052670-34-5 64

2 10.271 1.29 C:\Database\NIST98.L

2-Undecene, 4-methyl- 22861 1000061-82-8 46

2-Heptene, 4-methyl-, (E)- 22241 066225-17-0 38

Heptane, 4-methylene- 22748 015918-08-8 38

3 10.397 1.90 C:\Database\NIST98.L

Acetic acid, trifluoro-, 3,7-dimet 5224 028745-07-5 43

hyloctyl ester

5-Undecene, 3-methyl-, (Z)- 23873 074630-64-1 38

2-Undecene, 4-methyl- 22861 1000061-82-8 38

4 15.352 3.53 C:\Database\NIST98.L

Benzene, 1,3-bis(1,1-dimethylethyl 125075 001014-60-4 95

)-

Benzene, 1,3-bis(1,1-dimethylethyl 125073 001014-60-4 95

)-

m-Cymene, 5-tert-butyl- 75953 029577-19-3 86

5 16.748 2.35 C:\Database\NIST98.L

2-Acetylcyclopentanone 110242 001670-46-8 38

Hexane, 2,3,4-trimethyl- 6306 000921-47-1 38

Cyclohexane, 1,1,3,5-tetramethyl-, 23397 050876-31-8 30

trans-

6 16.977 2.45 C:\Database\NIST98.L

Cyclohexane, 1,1-dimethyl-2-propyl 22875 081983-71-3 49

3-Heptene, 2,2,3,5,6-pentamethyl- 23398 116164-06-8 35

Dibutyl-cyanamime 22840 1000144-08-0 35

7 17.206 1.84 C:\Database\NIST98.L

4-Isopropyl-1,3-cyclohexanedione 22410 062831-62-3 53

Cyclohexane, 1,1-dimethyl-2-propyl 22875 081983-71-3 49

2-Acetylcyclopentanone 8060 001670-46-8 38

8 21.618 0.98 C:\Database\NIST98.L

Docosane 16531 000629-97-0 86

Heptacosane 112354 000593-49-7 83

Pentacosane 17109 000629-99-2 78

9 22.058 2.13 C:\Database\NIST98.L

Phenol, 2,4-bis(1,1-dimethylethyl) 125782 000096-76-4 97

Phenol, 2,4-bis(1,1-dimethylethyl) 80518 000096-76-4 95

Phenol, 2,4-bis(1,1-dimethylethyl) 125776 000096-76-4 94

10 22.304 1.13 C:\Database\NIST98.L

3-Hexene, 2,3-dimethyl- 111655 007145-23-5 25

4-Nonene, 2,3,3-trimethyl-, (Z)- 22269 063830-68-2 25

Cyclohexane, 1,1,3,5-tetramethyl-, 114330 050876-32-9 25

cis-

11 22.699 1.66 C:\Database\NIST98.L

Dodecane 112318 000112-40-3 90

Tetratriacontane 16431 014167-59-0 64

Pentacosane 109667 000629-99-2 64

12 22.957 1.43 C:\Database\NIST98.L

Undecane, 5-methyl- 109657 001632-70-8 35

Octacosane 112312 000630-02-4 27

Pentacosane 109666 000629-99-2 27

13 27.374 1.00 C:\Database\NIST98.L

Bacchotricuneatin c 24581 066563-30-2 38

Cyclohexane, 1,1,3,5-tetramethyl-, 114330 050876-32-9 30

cis-

4-Nonene, 2,3,3-trimethyl-, (Z)- 22269 063830-68-2 30

14 27.792 1.41 C:\Database\NIST98.L

3-Heptene, 2,2,3,5,6-pentamethyl- 23398 116164-06-8 38

Cyclohexane, 1,2-diethyl-3-methyl- 22852 061141-80-8 38

Bacchotricuneatin c 24581 066563-30-2 35

15 27.969 1.09 C:\Database\NIST98.L

Bacchotricuneatin c 24581 066563-30-2 38

Hexatriacontane 112335 000630-06-8 35

2-Hexene, 4-ethyl-2,3-dimethyl- 22511 1000149-19-7 25

16 28.490 1.05 C:\Database\NIST98.L

Cyclohexane, 1,2,4-trimethyl- 22847 002234-75-5 45

Cyclohexane, 1-ethyl-2-propyl- 22848 062238-33-9 38

Cyclohexane, 1,2-diethyl-3-methyl- 22852 061141-80-8 38

17 30.962 1.31 C:\Database\NIST98.L

Docosane 16531 000629-97-0 80

Hexatriacontane 112334 000630-06-8 80

Octadecane, 1-iodo- 112388 000629-93-6 80

18 31.757 5.48 C:\Database\NIST98.L

n-Hexadecanoic acid 109985 000057-10-3 93

Pentadecanoic acid 114896 001002-84-2 76

n-Hexadecanoic acid 114901 000057-10-3 70

19 32.891 0.96 C:\Database\NIST98.L

Heneicosane 17094 000629-94-7 90

Heptadecane 112321 000629-78-7 83

Docosane 16531 000629-97-0 83

20 35.431 2.34 C:\Database\NIST98.L

Tetradecanoic acid 114897 000544-63-8 87

Octadecanoic acid 114902 000057-11-4 74

Octadecanoic acid 109986 000057-11-4 58

21 46.434 1.17 C:\Database\NIST98.L

Octadecanoic acid, 2-(acetyloxy)-1 9075 055401-62-2 53

-[(acetyloxy)methyl]ethyl ester

3-Methyl-2-hexene (c,t) 2494 1000113-13-1 18

Furan, 3-ethyl-2,5-dihydro- 22243 025409-04-5 18

22 46.525 3.18 C:\Database\NIST98.L

Octadecanoic acid, 2-(acetyloxy)-1 9075 055401-62-2 62

-[(acetyloxy)methyl]ethyl ester

Hexadecanoic acid, 2,3-bis(acetylo 70191 055268-70-7 46

xy)propyl ester

Eicosanoic acid, 2,3-bis(acetyloxy 9074 055429-67-9 45

)propyl ester

23 46.737 2.28 C:\Database\NIST98.L

Nonacosane 112560 000630-03-5 95

Nonahexacontanoic acid 17028 040710-32-5 91

Nonacosane 109621 000630-03-5 90

24 48.047 1.40 C:\Database\NIST98.L

Triacontane 17141 000638-68-6 96

Eicosane 112565 000112-95-8 93

Pentatriacontane 112346 000630-07-9 90

25 49.335 1.63 C:\Database\NIST98.L

Hentriacontane 112561 000630-04-6 93

Eicosane 112565 000112-95-8 83

Docosane 16531 000629-97-0 70

26 49.701 10.54 C:\Database\NIST98.L

Benzene, trichloro[(dichlorophenyl 70396 074421-51-5 12

)methoxy]-

4,4,6-Trimethyltetrahydro-1,3-oxaz 3786 017374-19-5 12

ine-2-thione

Cyclopropanecarboxylic acid, 1-(ph 70312 108546-70-9 10

enylmethyl)-, 2,6-bis(1,1-dimethyl

ethyl)-4-methylphenyl ester

27 49.798 31.70 C:\Database\NIST98.L

Oxazole, 5-methyl-2-phenyl- 124089 005221-67-0 32

3-Benzyl-1H-1,2,4-triazole 70350 021117-34-0 23

Cyclopropanecarboxylic acid, 1-(ph 70312 108546-70-9 9

enylmethyl)-, 2,6-bis(1,1-dimethyl

ethyl)-4-methylphenyl ester

28 50.577 1.28 C:\Database\NIST98.L

Eicosane 112565 000112-95-8 96

Eicosane 16454 000112-95-8 95

Octacosane 112312 000630-02-4 95

29 52.225 1.76 C:\Database\NIST98.L

.gamma.-Sitosterol 109486 000083-47-6 90

Ethyl 2-(2-chloroacetamido)-3,3,3- 84746 1000224-17-1 38

trifluoro-2-(3-fluoroanilino)propi

onate

1H-Indole, 5-methyl-2-phenyl- 84867 013228-36-9 27

30 53.918 8.32 C:\Database\NIST98.L

4-Benzoyl-N-(4-methylbenzylidene)- 106349 095855-26-8 45

3,5-diphenyl-2-furanamine

9-O-Pivaloyl-N-acetylcolchinol 106352 1000127-10-7 9

N-Acetoacetyl-deacetylcolchicine 10095 1000127-13-2 9

**EXTRACT CHCL3 WITH FILTER PVDF**

Data File : 191203001.D

Acq On : 3 Dec 2019 11:18 (#1); 03 Dec 2019 11:13 (#2)

Operator : KAREN MENDEZ

Sample : CHCL3 1:1 PVDF

Search Libraries: C:\Database\NIST98.L Minimum Quality: 0

Pk# RT Area% Library/ID Ref# CAS# Qual

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

1 9.401 0.53 C:\Database\NIST98.L

Benzene, 1-methyl-3-propyl- 119334 001074-43-7 38

Benzene, 1-methyl-3-propyl- 46925 001074-43-7 38

Benzene, (1-methylpropyl)- 119327 000135-98-8 35

2 10.454 2.27 C:\Database\NIST98.L

Benzene, 4-ethyl-1,2-dimethyl- 53592 000934-80-5 93

Benzene, 4-ethyl-1,2-dimethyl- 120817 000934-80-5 93

Benzene, 1-ethyl-2,3-dimethyl- 120813 000933-98-2 87

3 11.347 0.51 C:\Database\NIST98.L

1,3-Cyclopentadiene, 1,2,3,4-tetra 53597 076089-59-3 87

methyl-5-methylene-

Benzene, 1,2,4,5-tetramethyl- 53581 000095-93-2 81

Benzene, 1,2,3,4-tetramethyl- 120809 000488-23-3 81

4 11.473 0.82 C:\Database\NIST98.L

1,3-Cyclopentadiene, 1,2,3,4-tetra 53597 076089-59-3 95

methyl-5-methylene-

Benzene, 1,2,3,5-tetramethyl- 120821 000527-53-7 94

Benzene, 1,2,3,4-tetramethyl- 120809 000488-23-3 94

5 13.327 0.91 C:\Database\NIST98.L

Azulene 57920 000275-51-4 49

Naphthalene 121778 000091-20-3 49

Naphthalene 121777 000091-20-3 49

6 14.276 0.43 C:\Database\NIST98.L

Cycloheptanol, 2-chloro-, trans- 18516 069578-07-0 32

2-Nonanone, 9-[(tetrahydro-2H-pyra 7100 054699-41-1 12

n-2-yl)oxy]-

2-Penten-4-yn-1-ol, 3-methyl-, (E) 31923 006153-06-6 11

7 14.534 5.33 C:\Database\NIST98.L

Benzothiazole 122345 000095-16-9 95

Benzothiazole 122346 000095-16-9 87

1,2-Benzisothiazole 61206 000272-16-2 86

8 14.706 2.49 C:\Database\NIST98.L

2-Butenal, 3-methyl- 33657 000107-86-8 25

2-Cyclohexen-1-one, 4-(3-hydroxy-1 48986 052210-15-8 14

-butenyl)-3,5,5-trimethyl-, [r-[r\*

,R\*-(E)]]-

Furan, 2,3-dihydro-5-methyl- 110041 001487-15-6 14

9 16.130 0.62 C:\Database\NIST98.L

(Cyclopropyl)trivinylsilane 49218 1000109-93-8 27

Cyclohexanepropanol- 111605 001124-63-6 23

Cyclopropane, trimethylmethylene- 116046 034462-28-7 22

10 16.525 0.43 C:\Database\NIST98.L

Cyclohexanol, 2,4-dimethyl- 41022 069542-91-2 22

3-Octyne, 6-methyl- 1500 062108-34-3 22

Pentaleno[1,2-b]oxirene, octahydro 41181 055449-71-3 11

-, (1a.alpha.,1b.alpha.,4a.beta.,5

a.alpha.)-

11 17.652 0.74 C:\Database\NIST98.L

Cyclopentanone, 3-methyl-2-(2-pent 33269 007051-39-0 38

enyl)-

Cyclopropanol, 1-(3,7-dimethyl-1-o 32872 065147-72-0 35

ctenyl)-

E-11(13,13-Dimethyl)tetradecen-1-o 32808 1000130-80-2 25

l acetate

12 18.001 0.42 C:\Database\NIST98.L

Pentyl acetoacetate 109842 006624-84-6 32

Undecanal, 2-methyl- 18534 000110-41-8 27

Undecanal 1770 000112-44-7 25

13 18.122 1.62 C:\Database\NIST98.L

Cyclopentanecarboxylic acid, 3-met 33265 1000152-25-8 35

hyl-4-methylene-, menthyl ester

Bicyclo[2.2.1]heptane, 2,2,3-trime 41434 000473-19-8 30

thyl-

2-Pentenal, (E)- 14368 001576-87-0 27

14 18.591 0.45 C:\Database\NIST98.L

Phytol 114590 000150-86-7 42

Cyclohexanol, 3,5-dimethyl- 114635 005441-52-1 37

Propanoic acid, 2-methyl-, 2,2-dim 24402 074367-33-2 37

ethyl-1-(2-hydroxy-1-methylethyl)p

ropyl ester

15 19.873 1.80 C:\Database\NIST98.L

Isocitronellol 32843 1000149-89-1 38

Ethyl trans-2-pentenoate 33011 024410-84-2 38

(E)-2-Hexenyl tiglate 32840 1000131-83-6 32

16 20.153 0.57 C:\Database\NIST98.L

3-Cyclopropenoic acid,-1-butyl, me 1371 1000222-93-4 35

thyl ester

3-Hepten-2-one, 5-methyl- 13501 005090-16-4 27

2,4-Dimethyl-1-heptene 6200 019549-87-2 27

17 20.880 1.70 C:\Database\NIST98.L

Heptylcyclohexane 33188 005617-41-4 49

Hexane, 1,6-dibromo- 116394 000629-03-8 35

2-Hexene, 4,4,5-trimethyl- 32878 055702-61-9 35

18 21.080 1.03 C:\Database\NIST98.L

Oxirane, tetradecyl- 108844 007320-37-8 27

1-Octadecanol 111484 000112-92-5 22

5-Octadecene, (E)- 13707 007206-21-5 18

19 21.784 0.64 C:\Database\NIST98.L

4H-4a,7-Methanooxazirino[3,2-I][2, 2841 104322-63-6 25

1]benzisothiazole, tetrahydro-9,9-

dimethyl-, 3,3-dioxide, [4as-(4a.a

lpha.,7.alpha.,8ar\*)]-

2(3H)-Naphthalenone, 4,4a,5,6,7,8- 1877 004087-39-2 22

hexahydro-4a-methyl-, (S)-

2-Hexyn-1-ol 1547 000764-60-3 22

20 22.064 3.25 C:\Database\NIST98.L

Phenol, 2,4-bis(1,1-dimethylethyl) 125782 000096-76-4 95

Phenol, 2,4-bis(1,1-dimethylethyl) 80518 000096-76-4 93

Phenol, 2,6-bis(1,1-dimethylethyl) 80511 000128-39-2 91

21 22.705 0.58 C:\Database\NIST98.L

2H-Pyran-2-one, 6-hexyltetrahydro- 118536 000710-04-3 59

2-Pyrrolidinone, 1-methyl- 43090 000872-50-4 52

trans-4-Hydroxy-3-methylundecanoic 43003 148806-10-4 45

acid lactone

22 23.071 0.63 C:\Database\NIST98.L

Cyclohexane, nitro- 111373 001122-60-7 35

2H-Quinolizine-1-carboxylic acid, 33280 000574-99-2 30

octahydro-, (1R-trans)-

2-(Prop-2-enoyloxy)tetradecane 13005 1000245-67-0 27

23 24.038 0.90 C:\Database\NIST98.L

Diethyl Phthalate 123514 000084-66-2 58

Diethyl Phthalate 67077 000084-66-2 53

1,2-Benzenedicarboxylic acid, mono 67064 004376-20-9 50

(2-ethylhexyl) ester

24 27.111 0.68 C:\Database\NIST98.L

(4-Fluorophenyl)acetone 110368 000459-03-0 35

Cyclohexanol, 1-methyl-4-(1-methyl 24621 021129-27-1 27

ethyl)-

2H-Inden-2-one, octahydro-3a-methy 41139 020379-99-1 25

l-, trans-

25 28.433 0.42 C:\Database\NIST98.L

4.Xi.-Germacr-9-en-12-oic acid, 6. 41075 019906-69-5 38

alpha.-hydroxy-1-oxo-, .gamma.-lac

tone, (11S)-

2-Hexen-1-ol, 2-ethyl- 111483 050639-00-4 38

D-Streptamine, O-2-amino-2-deoxy-. 3335 007542-37-2 37

alpha.-D-glucopyranosyl-(14)-O-[O-

2,6-diamino-2,6-dideoxy-.beta.-L-i

dopyranosyl-(13)-.beta.-D-ribofura

nosyl-(15)]-2-deoxy-

26 28.644 0.67 C:\Database\NIST98.L

Bicyclo[2.2.2]octane-2,6-dione 14753 038231-60-6 22

3,10-Dioxatricyclo[4.3.1.0(2,4)]de 8756 038314-22-6 22

can-7-ol, acetate, (1.alpha.,2.alp

ha.,4.alpha.,6.alpha.,7.beta.)-

Hexahydro-pentalene-1,6-dione 62653 090953-74-5 8

27 30.092 0.67 C:\Database\NIST98.L

5-Octadecene, (E)- 13707 007206-21-5 78

1-Octadecanol 111484 000112-92-5 64

3-Octadecene, (E)- 22895 007206-19-1 60

28 30.956 1.61 C:\Database\NIST98.L

7,9-Di-tert-butyl-1-oxaspiro(4,5)d 17969 1000143-92-4 50

eca-6,9-diene-2,8-dione

2,4-Dimethyl-5,6-dimethoxy-8-amino 86997 1000213-45-0 38

quinoline

Ethanone, 1,1'-(6-methoxy-2,5-benz 87050 023840-15-5 35

ofurandiyl)bis-

29 31.019 1.10 C:\Database\NIST98.L

Pentadecanoic acid, 14-methyl-, me 115450 005129-60-2 93

thyl ester

Hexadecanoic acid, methyl ester 115419 000112-39-0 93

Hexadecanoic acid, methyl ester 115367 000112-39-0 87

30 31.391 0.49 C:\Database\NIST98.L

Imidazolo[3,4-d]-1,4-diazepine, 7- 96877 1000211-47-1 18

phenylsulfonyl-5,6,8,9(7H)-tetrahy

dro-

8H-Naphtho[1,2-b]pyran-8-one, 3-et 9947 055836-76-5 16

hyldodecahydro-3,4a,7,7,10a-pentam

ethyl-, [3R-(3.alpha.,4a.beta.,6a.

alpha.,10a.beta.,10b.alpha.)]-

2-Methoxy-5-amino-4,6-diphenylpyri 96914 076891-83-3 14

midine

31 31.706 6.72 C:\Database\NIST98.L

Tridecanoic acid 114895 000638-53-9 89

n-Hexadecanoic acid 114901 000057-10-3 86

n-Hexadecanoic acid 109985 000057-10-3 72

32 32.432 0.57 C:\Database\NIST98.L

Guanidineacetic acid 7625 000352-97-6 43

2H-Pyran-2-one, tetrahydro-6-penty 43208 000705-86-2 38

l-

2H-Pyran-2-one, tetrahydro-6-nonyl 43191 002721-22-4 38

33 33.989 1.65 C:\Database\NIST98.L

9-Octadecene, (E)- 13709 007206-25-9 89

1-Heptadecanol 13564 001454-85-9 70

1-Eicosanol 112640 000629-96-9 70

34 34.206 0.65 C:\Database\NIST98.L

9,12-Octadecadienoic acid (Z,Z)-, 116129 000112-63-0 96

methyl ester

9,12-Octadecadienoic acid, methyl 21420 002462-85-3 90

ester

9,12-Octadecadienoic acid (Z,Z)- 113793 000060-33-3 87

35 34.315 0.45 C:\Database\NIST98.L

2-Methyl-Z,Z-3,13-octadecadienol 12982 1000130-90-5 53

Eicosenoic acid, methyl ester 4281 027070-40-2 46

9-Octadecene, (E)- 13709 007206-25-9 38

36 34.784 0.97 C:\Database\NIST98.L

Heptadecanoic acid, 16-methyl-, me 28391 005129-61-3 98

thyl ester

Octadecanoic acid, methyl ester 115467 000112-61-8 93

Octadecanoic acid, methyl ester 28371 000112-61-8 93

37 34.881 0.58 C:\Database\NIST98.L

Tridecanedial 14456 063521-76-6 62

9-Eicosyne 31672 071899-38-2 52

9-Octadecyne 116116 035365-59-4 50

38 34.973 0.84 C:\Database\NIST98.L

Aspidospermidin-17-ol, 1-acetyl-19 22983 002122-26-1 52

,21-epoxy-15,16-dimethoxy-

Cyclopentane, 1,1'-[3-(2-cyclopent 2576 055255-85-1 43

ylethyl)-1,5-pentanediyl]bis-

4-Heptadecenal 16588 1000143-91-7 40

39 35.104 0.92 C:\Database\NIST98.L

Hexadecanoic acid, 1,1-dimethyleth 15255 031158-91-5 35

yl ester

1-Undecene, 5-methyl- 15134 074630-38-9 22

2-Hexene, 5-methyl-, (E)- 15211 007385-82-2 14

40 35.408 4.45 C:\Database\NIST98.L

Octadecanoic acid 114902 000057-11-4 98

Heptadecanoic acid 114893 000506-12-7 64

Octadecanoic acid 109378 000057-11-4 62

41 35.843 4.83 C:\Database\NIST98.L

Hexadecanoic acid, 1,1-dimethyleth 15255 031158-91-5 96

yl ester

Hexadecanoic acid, butyl ester 15257 000111-06-8 87

Eicosanoic acid 109983 000506-30-9 25

42 36.249 0.55 C:\Database\NIST98.L

Phosphonic acid, dioctadecyl ester 13890 019047-85-9 53

1-Heptadecanol 13564 001454-85-9 52

Trifluoroacetic acid, n-tetradecyl 4218 1000216-79-0 49

ester

43 37.748 0.47 C:\Database\NIST98.L

Tetratriacontane 16431 014167-59-0 49

Tetratetracontane 112365 007098-22-8 46

Hexatriacontane 112334 000630-06-8 46

44 39.213 3.10 C:\Database\NIST98.L

Octadecanoic acid, butyl ester 111934 000123-95-5 93

Octadecanoic acid, butyl ester 15286 000123-95-5 91

Octadecanoic acid, 2-methylpropyl 16846 000646-13-9 87

ester

45 39.396 0.92 C:\Database\NIST98.L

Heptacosane 16471 000593-49-7 90

Tetratriacontane 16431 014167-59-0 90

Docosane 16531 000629-97-0 87

46 40.964 0.93 C:\Database\NIST98.L

Tetratetracontane 16486 007098-22-8 83

Tetrapentacontane 112596 005856-66-6 80

Heptacosane 16471 000593-49-7 74

47 41.765 0.64 C:\Database\NIST98.L

1,2-Benzenedicarboxylic acid, diis 123512 027554-26-3 59

ooctyl ester

Bis(2-ethylhexyl) phthalate 66784 000117-81-7 59

Bis(2-ethylhexyl) phthalate 123452 000117-81-7 53

48 42.486 1.34 C:\Database\NIST98.L

Tetratriacontane 16431 014167-59-0 76

Tetrapentacontane, 1,54-dibromo- 17122 1000156-09-4 68

Eicosane 112565 000112-95-8 68

49 43.665 0.84 C:\Database\NIST98.L

Stannane, iodotripropyl- 84807 007342-45-2 25

Acetic acid, 4-(3-acetylamino-2-ox 933 1000194-74-7 22

opropyl)phenyl ester

1,2,4-Triazin-3(2H)-one, 5,6-diphe 92921 004512-00-9 22

nyl-

50 43.945 0.96 C:\Database\NIST98.L

Eicosane 16454 000112-95-8 95

Eicosane 112565 000112-95-8 55

Heptadecane 16420 000629-78-7 53

51 44.220 0.62 C:\Database\NIST98.L

Silicic acid, diethyl bis(trimethy 84851 003555-45-1 38

lsilyl) ester

Hexahydropyridine, 1-methyl-4-[4,5 84723 094427-47-1 35

-dihydroxyphenyl]-

4-Heptafluorobutyroxypentadecane 12999 1000245-50-2 18

52 45.106 1.04 C:\Database\NIST98.L

9-Octadecenamide, (Z)- 19657 000301-02-0 60

Erucylamide 19656 000112-84-5 46

9-Octadecenamide, (Z)- 113302 000301-02-0 46

53 45.370 1.18 C:\Database\NIST98.L

Eicosane 112565 000112-95-8 95

Eicosane 16454 000112-95-8 87

Nonadecane 112381 000629-92-5 53

54 45.810 4.80 C:\Database\NIST98.L

2,6,10,14,18-Pentamethyl-2,6,10,14 23038 075581-03-2 74

,18-eicosapentaene

Squalene 114269 007683-64-9 68

1,6,10,14,18,22-Tetracosahexaen-3- 23039 054159-46-5 64

ol, 2,6,10,15,19,23-hexamethyl-, (

all-E)-

55 46.720 1.47 C:\Database\NIST98.L

Octadecane 16439 000593-45-3 83

Eicosane 112565 000112-95-8 46

Ethanol, 2-(octadecyloxy)- 16507 002136-72-3 46

56 48.053 1.59 C:\Database\NIST98.L

Eicosane 112565 000112-95-8 40

Heptacosane, 1-chloro- 16427 062016-79-9 18

6-Azaestra-1,3,5(10),6,8-pentaen-1 97338 005144-20-7 18

7-one, 3-methoxy-

57 48.997 2.69 C:\Database\NIST98.L

N-Methyl-1-adamantaneacetamide 84775 1000211-60-4 50

N-Cyano-N',N',N'',N''-tetramethyl- 84777 074150-88-2 38

1,3,5-triazinetriamine

Cyclotrisiloxane, hexamethyl- 84874 000541-05-9 25

58 49.272 6.12 C:\Database\NIST98.L

Stigmastan-3,5-dien 10351 1000214-16-4 47

1H-Indole, 5-methyl-2-phenyl- 84867 013228-36-9 22

Cyclotrisiloxane, hexamethyl- 126481 000541-05-9 22

59 52.219 13.80 C:\Database\NIST98.L

Stigmastan-3,5-dien 10351 1000214-16-4 60

1-Propene, 3-(2-cyclopentenyl)-2-m 84768 1000154-23-3 45

ethyl-1,1-diphenyl-

Stigmast-5-en-3-ol, oleate 105236 1000154-66-5 25

**EXTRACT CHCl3 WITH FILTER PTFE**

Data File : 191203002.D

Acq On : 3 Dec 2019 14:59 (#1); 03 Dec 2019 14:54 (#2)

Operator : KAREN MENDEZ

Sample : CHCL3 1:1 PTFE

Search Libraries: C:\Database\NIST98.L Minimum Quality: 0

Pk# RT Area% Library/ID Ref# CAS# Qual

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1 5.127 0.93 C:\Database\NIST98.L

1,3-Cyclopentadiene, 5-(1-methylet 37691 002175-91-9 9

hylidene)-

1-Cycloocten-5-yne, (Z)- 36595 066633-23-6 9

Benzene, 1,2-dimethyl- 117410 000095-47-6 9

2 9.453 1.31 C:\Database\NIST98.L

1(3H)-Isobenzofuranone 45966 000087-41-2 4

1(3H)-Isobenzofuranone 119138 000087-41-2 4

Oxirane, 2-methyl-2-phenyl- 119325 002085-88-3 4

3 10.259 2.51 C:\Database\NIST98.L

Benzene, 2-ethyl-1,3-dimethyl- 120726 002870-04-4 64

Benzene, 1-ethyl-2,3-dimethyl- 120728 000933-98-2 64

Benzene, 1-ethyl-2,4-dimethyl- 120736 000874-41-9 64

4 10.454 4.24 C:\Database\NIST98.L

Benzene, 1-ethyl-2,3-dimethyl- 53590 000933-98-2 80

Benzene, 4-ethyl-1,2-dimethyl- 53592 000934-80-5 80

Benzene, 2-ethyl-1,3-dimethyl- 120726 002870-04-4 72

5 11.370 1.75 C:\Database\NIST98.L

Ethanone, 1-(4-methylphenyl)- 120732 000122-00-9 5

Benzene, 1,3-diethyl- 120774 000141-93-5 5

Acetonitrile, bromo- 108421 000590-17-0 2

6 11.484 0.83 C:\Database\NIST98.L

Benzene, 2-ethyl-1,3-dimethyl- 53585 002870-04-4 74

Benzene, 4-ethyl-1,2-dimethyl- 53592 000934-80-5 74

Benzene, 1-ethyl-2,4-dimethyl- 120822 000874-41-9 9

7 14.562 1.95 C:\Database\NIST98.L

1,2,4-Dithiazole-3-thione 60861 1000105-35-6 5

p-Benzoquinone 111113 000106-51-4 4

p-Benzoquinone 111178 000106-51-4 4

8 21.640 1.04 C:\Database\NIST98.L

Cyclobutanone, oxime 17299 002972-05-6 4

Cyclobutanone, oxime 112649 002972-05-6 4

Acetamide, N-ethenyl-N-methyl- 16858 003195-78-6 4

9 22.070 5.28 C:\Database\NIST98.L

Phenol, bis(1,1-dimethylethyl)- 80741 026746-38-3 83

Phenol, 2,4-bis(1,1-dimethylethyl) 125781 000096-76-4 83

Phenol, 2,4-bis(1,1-dimethylethyl) 125782 000096-76-4 78

10 26.567 0.89 C:\Database\NIST98.L

Hexane, 2,3,4-trimethyl- 6306 000921-47-1 9

2-Propenamide 114463 000079-06-1 4

2-Propenamide 24220 000079-06-1 4

11 31.723 1.65 C:\Database\NIST98.L

Propanamide 110481 000079-05-0 4

1-Methoxy-5-trifluoroacetoxyhexane 11659 1000216-63-2 4

Guanidine, methyl- 108192 000471-29-4 3

12 34.801 1.87 C:\Database\NIST98.L

Methyl 7-methylhexadecanoate 28213 018720-85-9 40

Methyl 8-oxooctanoate 2691 004316-48-7 28

Decanoic acid, 8-methyl-, methyl e 28380 005129-64-6 9

ster

13 35.121 2.49 C:\Database\NIST98.L

1-Dodecanol, 2-methyl-, (S)- 15951 057289-26-6 38

2-Methyl-1-undecanol 16300 010522-26-6 38

Hexadecanoic acid, 1,1-dimethyleth 15255 031158-91-5 25

yl ester

14 35.425 1.19 C:\Database\NIST98.L

.alpha.-D-Galactopyranoside, methy 17188 005540-31-8 23

l 3,6-anhydro-

4-Fluorohistamine 10678 049872-60-8 7

2-Acetyl-2-thiazoline 5930 1000121-56-5 5

15 35.848 23.01 C:\Database\NIST98.L

Hexadecanoic acid, butyl ester 15257 000111-06-8 98

Hexadecanoic acid, 1,1-dimethyleth 15255 031158-91-5 92

yl ester

1-Hexene, 2,5-dimethyl- 15038 006975-92-4 25

16 36.260 1.20 C:\Database\NIST98.L

Cyclohexane, 1-(1,5-dimethylhexyl) 5219 056009-20-2 53

-4-(4-methylpentyl)-

1-Octadecene 112297 000112-88-9 50

Undecane, 3-cyclohexyl- 17256 013151-78-5 38

17 37.027 0.78 C:\Database\NIST98.L

Ethane, isothiocyanato- 116954 000542-85-8 2

Vanadium, (.eta.7-cycloheptatrieny 126462 012636-68-9 2

lium)(.eta.5-2,4-cyclopentadien-1-

yl)-

2-Propanone, O-methyloxime 116951 003376-35-0 2

18 38.537 1.37 C:\Database\NIST98.L

9-Borabicyclo[3.3.1]nonane, 9-[3-( 84721 1000160-35-2 5

dimethylamino)propyl]-

Hexahydropyridine, 1-methyl-4-[4,5 84723 094427-47-1 5

-dihydroxyphenyl]-

Azetidine, 1-methyl- 119 004923-79-9 4

19 39.224 10.83 C:\Database\NIST98.L

Octadecanoic acid, butyl ester 111934 000123-95-5 94

Octadecanoic acid, butyl ester 111935 000123-95-5 93

Octadecanoic acid, 2-methylpropyl 16846 000646-13-9 90

ester

20 39.407 4.95 C:\Database\NIST98.L

1-Decanol, 2-hexyl- 112269 002425-77-6 43

Bacchotricuneatin c 24581 066563-30-2 38

Dodecane, 1-fluoro- 16780 000334-68-9 35

21 39.579 0.76 C:\Database\NIST98.L

Hexahydropyridine, 1-methyl-4-[4,5 84723 094427-47-1 5

-dihydroxyphenyl]-

N-Methyl-1-adamantaneacetamide 84775 1000211-60-4 5

cis-4-Ethoxy-b-methyl-b-nitrostyre 84793 1000120-36-6 4

ne

22 40.981 1.43 C:\Database\NIST98.L

Ethanol, 2-(hexadecyloxy)- 112374 002136-71-2 27

Nonahexacontanoic acid 17028 040710-32-5 27

Ethanol, 2-(dodecyloxy)- 16546 004536-30-5 27

23 41.490 0.80 C:\Database\NIST98.L

7-Chloro-4-methoxy-3-methylquinoli 84815 1000213-52-2 5

ne

Dodecahydropyrido[1,2-b]isoquinoli 84738 1000195-30-7 5

n-6-one

Pyrido[2,3-d]pyrimidine, 4-phenyl- 84862 028732-75-4 5

24 41.770 7.55 C:\Database\NIST98.L

1,2-Benzenedicarboxylic acid, mono 123456 004376-20-9 53

(2-ethylhexyl) ester

Bis(2-ethylhexyl) phthalate 66784 000117-81-7 43

1,2-Benzenedicarboxylic acid, mono 67064 004376-20-9 40

(2-ethylhexyl) ester

25 41.976 0.77 C:\Database\NIST98.L

Indole-2-one, 2,3-dihydro-N-hydrox 84802 1000129-52-1 5

y-4-methoxy-3,3-dimethyl-

9-Borabicyclo[3.3.1]nonane, 9-[3-( 84721 1000160-35-2 5

dimethylamino)propyl]-

3,5-Dimethylbenzaldehyde thiocarba 84771 1000195-15-1 5

moylhydrazone

26 42.491 1.75 C:\Database\NIST98.L

Cyclopenteno[4.3-b]tetrahydrofuran 84789 1000211-22-7 33

, 3-[(4-methyl-5-oxo-3-phenylthio)

tetrahydrofuran-2-yloxymethylene]-

N-(2-Acetylcyclopentylidene)cycloh 84801 1000100-48-5 9

exylamine

9-Borabicyclo[3.3.1]nonane, 9-[3-( 84721 1000160-35-2 9

dimethylamino)propyl]-

27 49.346 16.87 C:\Database\NIST98.L

Silicic acid, diethyl bis(trimethy 84851 003555-45-1 42

lsilyl) ester

Arsenous acid, tris(trimethylsilyl 84872 055429-29-3 38

) ester

Cyclotrisiloxane, hexamethyl- 126481 000541-05-9 38