LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\
Data File : BF118295.D
Acq On : 19 Dec 2019 22:40
Operator : JU
Sample : K6325-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT-3860

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.063 | 502 | 506 | 516 | rVB | 318654 | 390064 | 13.79% | 1.548% |
| 2 | 5.475 | 572 | 576 | 600 | rBV | 2331079 | 2163400 | 76.51% | 8.584% |
| 3 | 6.134 | 685 | 688 | 691 | rBV | 55173 | 42555 | 1.50% | 0.169% |
| 4 | 6.493 | 744 | 749 | 758 | rBV | 2216055 | 2283717 | 80.77% | 9.061% |
| 5 | 6.557 | 758 | 760 | 768 | rVB | 42042 | 36852 | 1.30% | 0.146% |
| 6 | 6.628 | 768 | 772 | 775 | rBV | 2962097 | 2454113 | 86.79% | 9.737% |
| 7 | 6.857 | 807 | 811 | 820 | rBV | 741939 | 591434 | 20.92% | 2.347% |
| 8 | 7.016 | 834 | 838 | 841 | rBV | 2207367 | 1896628 | 67.08% | 7.525% |
| 9 | 7.422 | 903 | 907 | 919 | rBV | 1536269 | 1418229 | 50.16% | 5.627% |
| 10 | 8.145 | 1026 | 1030 | 1045 | rBV | 795073 | 753045 | 26.63% | 2.988% |
| 11 | 9.222 | 1209 | 1213 | 1216 | rBV | 3335124 | 2642755 | 93.46% | 10.486% |
| 12 | 9.557 | 1267 | 1270 | 1273 | rBV | 45857 | 33666 | 1.19% | 0.134% |
| 13 | 9.616 | 1277 | 1280 | 1290 | rBV | 103519 | 116110 | 4.11% | 0.461% |
| 14 | 9.904 | 1326 | 1329 | 1340 | rVB | 1052263 | 922009 | 32.61% | 3.658% |
| 15 | 10.698 | 1460 | 1464 | 1474 | rBV | 2040969 | 1934076 | 68.40% | 7.674% |
| 16 | 11.398 | 1579 | 1583 | 1586 | rBV | 1073579 | 929096 | 32.86% | 3.686% |
| 17 | 11.922 | 1667 | 1672 | 1680 | rBV2 | 263386 | 287696 | 10.17% | 1.142% |
| 18 | 12.016 | 1685 | 1688 | 1699 | rVB | 31375 | 47595 | 1.68% | 0.189% |
| 19 | 12.616 | 1787 | 1790 | 1800 | rBV | 249343 | 241614 | 8.54% | 0.959% |
| 20 | 12.710 | 1803 | 1806 | 1812 | rBV2 | 43407 | 54531 | 1.93% | 0.216% |
| 21 | 12.851 | 1824 | 1830 | 1833 | rBV | 142434 | 169341 | 5.99% | 0.672% |
| 22 | 12.986 | 1849 | 1853 | 1856 | rBV | 3182350 | 2827598 | 100.00% | 11.219% |
| 23 | 13.557 | 1945 | 1950 | 1952 | rBV2 | 29676 | 32013 | 1.13% | 0.127% |
| 24 | 13.880 | 2002 | 2005 | 2018 | rVB | 344208 | 459354 | 16.25% | 1.823% |
| 25 | 14.051 | 2030 | 2034 | 2042 | rBV | 806709 | 808899 | 28.61% | 3.209% |
| 26 | 14.204 | 2056 | 2060 | 2066 | rBV | 50267 | 59856 | 2.12% | 0.237% |
| 27 | 14.510 | 2108 | 2112 | 2124 | rBV2 | 68019 | 109849 | 3.88% | 0.436% |
| 28 | 14.816 | 2160 | 2164 | 2171 | rBV | 71284 | 76998 | 2.72% | 0.306% |
| 29 | 14.892 | 2173 | 2177 | 2182 | rVB | 55800 | 56603 | 2.00% | 0.225% |
| 30 | 15.104 | 2209 | 2213 | 2216 | rBV2 | 23360 | 32509 | 1.15% | 0.129% |
| 31 | 15.163 | 2219 | 2223 | 2227 | rVB | 93373 | 110226 | 3.90% | 0.437% |
| 32 | 15.539 | 2282 | 2287 | 2298 | rBV2 | 551209 | 787481 | 27.85% | 3.125% |
| 33 | 15.992 | 2359 | 2364 | 2369 | rBV | 76788 | 113600 | 4.02% | 0.451% |
| 34 | 16.051 | 2369 | 2374 | 2383 | rBV4 | 59271 | 144709 | 5.12% | 0.574% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\
Data File : BF118295.D
Acq On : 19 Dec 2019 22:40
Operator : JU
Sample : K6325-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT-3860

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 16.504 | 2447 | 2451 | 2455 | rBV3 | 27421 | 47864 | 1.69% | 0.190% |
| 36 | 17.109 | 2550 | 2554 | 2561 | rVB5 | 19685 | 36479 | 1.29% | 0.145% |
| 37 | 17.633 | 2637 | 2643 | 2650 | rBV7 | 16903 | 43207 | 1.53% | 0.171% |
| 38 | 18.656 | 2812 | 2817 | 2828 | rVB9 | 18118 | 47501 | 1.68% | 0.188% |

Sum of corrected areas: 25203272

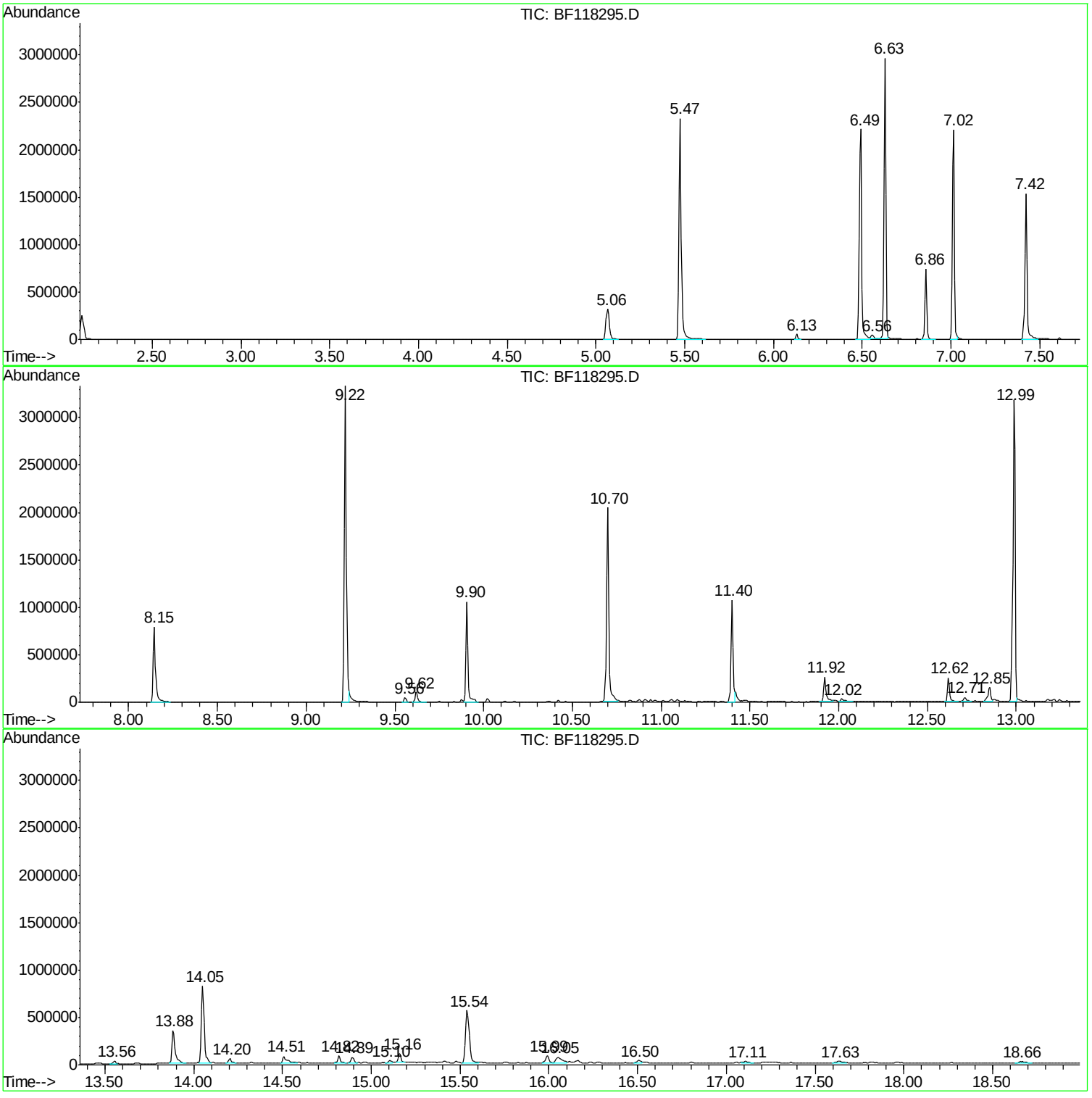
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\
Data File : BF118295.D
Acq On : 19 Dec 2019 22:40
Operator : JU
Sample : K6325-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT-3860

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\
Data File : BF118295.D
Acq On : 19 Dec 2019 22:40
Operator : JU
Sample : K6325-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT-3860

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

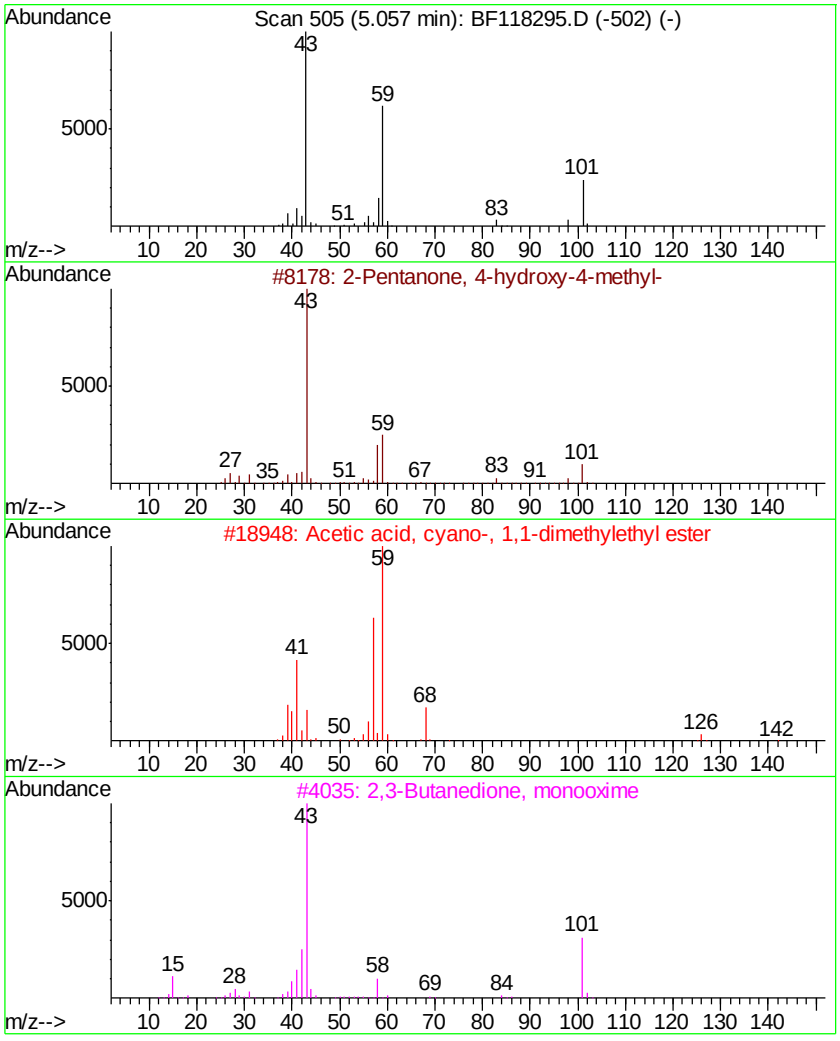
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

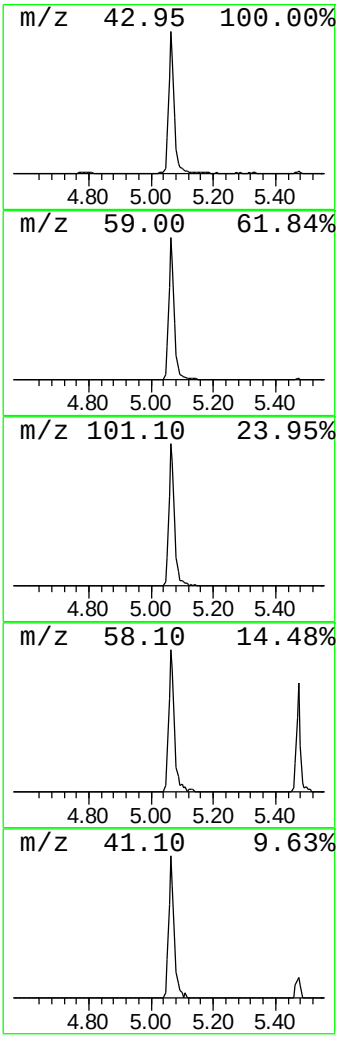
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.06 | 13.19 ng | 390064 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 17 |
| 4 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 5 | (+-)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\
Data File : BF118295.D
Acq On : 19 Dec 2019 22:40
Operator : JU
Sample : K6325-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT-3860

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

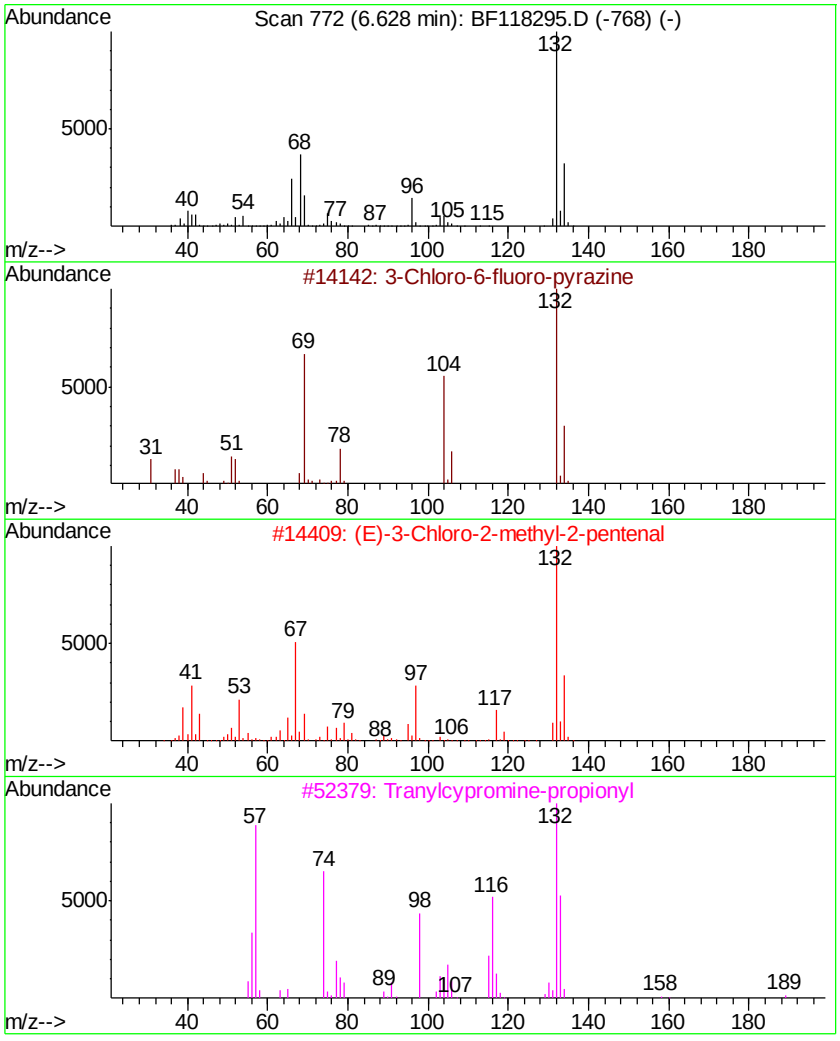
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

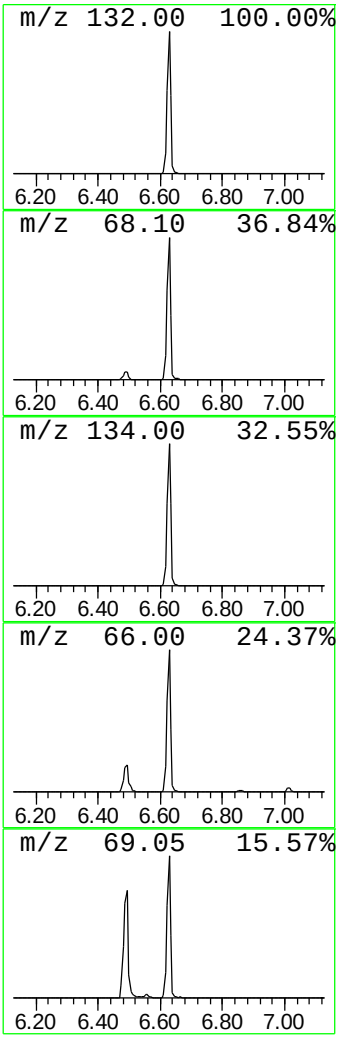
**********

Peak Number 2 unknown6.63 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.63 | 82.99 ng | 2454110 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 35 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 25 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 16 |
| 4 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 5 | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2 | 022291-85-6 | 9 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\
Data File : BF118295.D
Acq On : 19 Dec 2019 22:40
Operator : JU
Sample : K6325-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT-3860

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

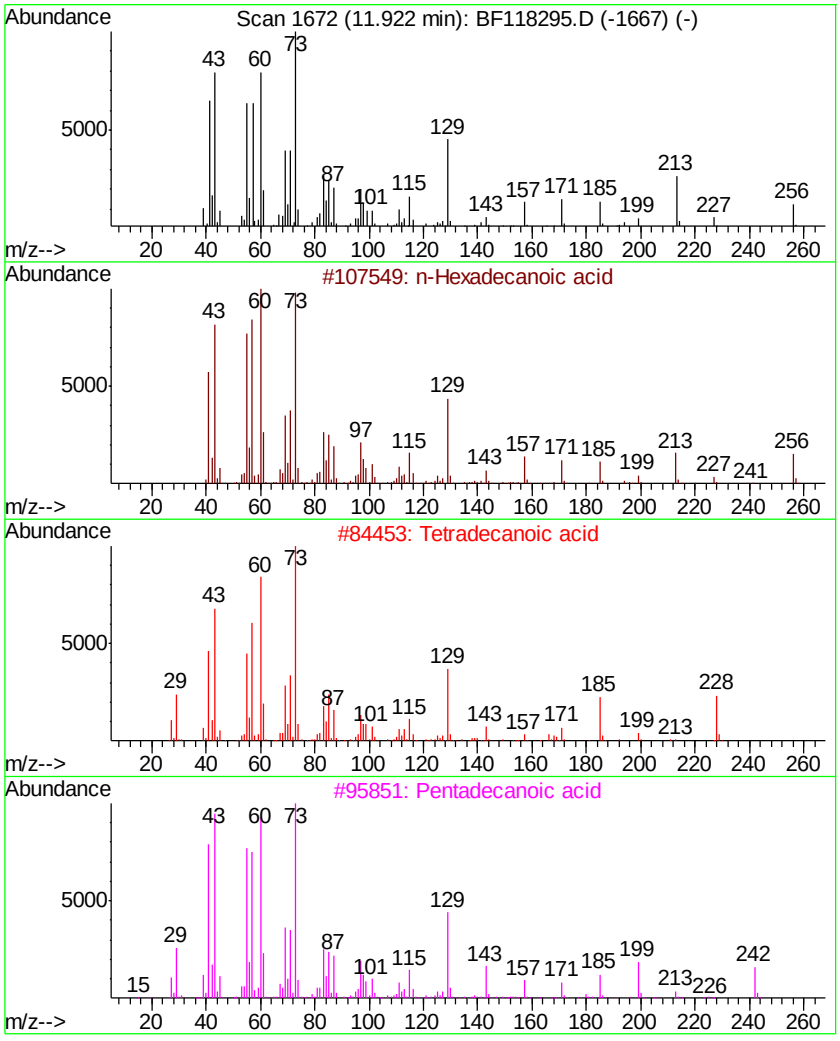
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

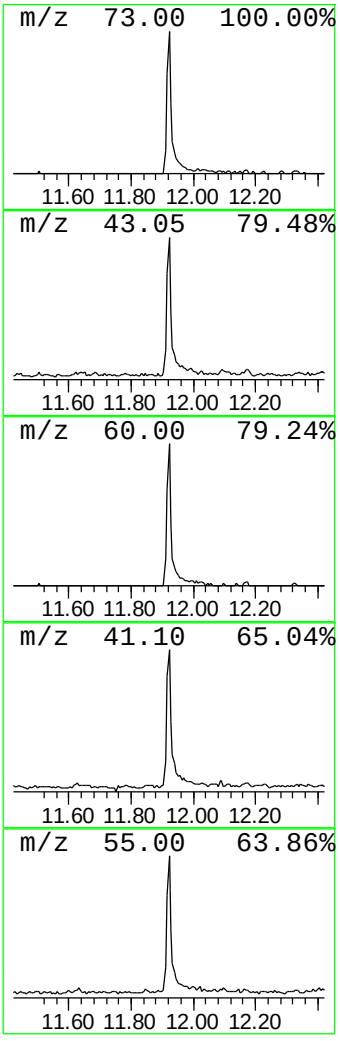
**********

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.92 | 6.19 ng | 287696 | Phenanthrene-d10 | 11.40 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 93 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 90 |
| 4 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 76 |
| 5 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 64 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\
Data File : BF118295.D
Acq On : 19 Dec 2019 22:40
Operator : JU
Sample : K6325-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT-3860

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

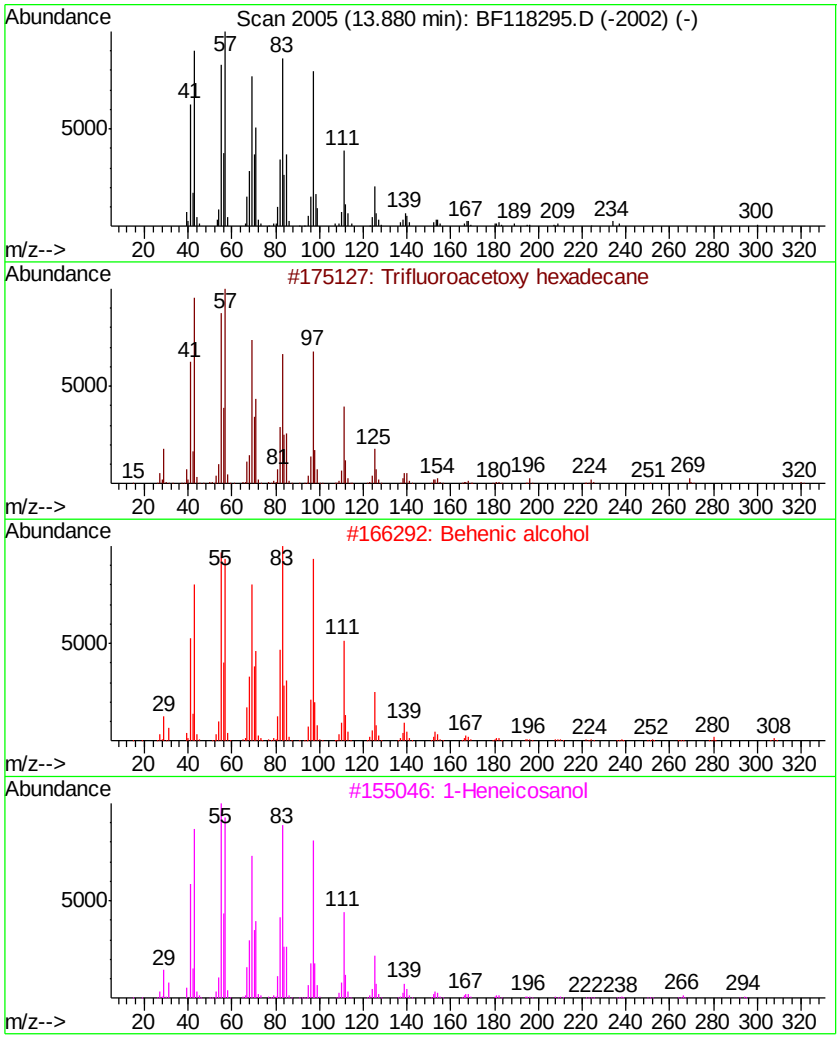
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

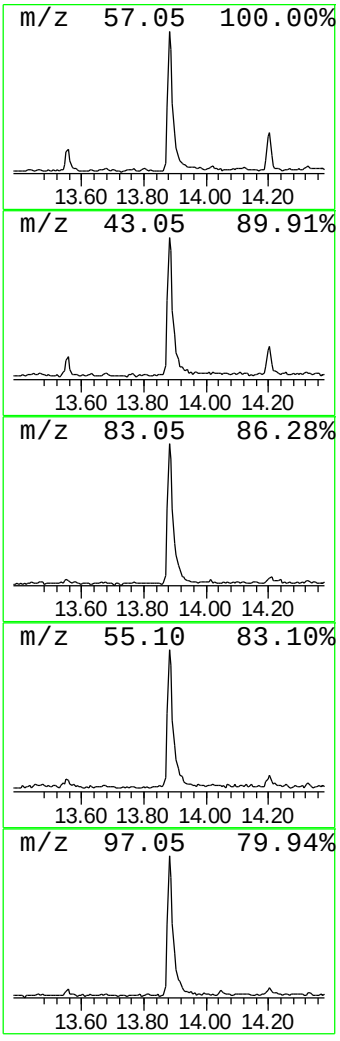
**********

Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.88 | 11.36 ng | 459354 | Chrysene-d12 | 14.05 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 94 |
| 2 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 93 |
| 3 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 93 |
| 4 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 93 |
| 5 | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 91 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\
Data File : BF118295.D
Acq On : 19 Dec 2019 22:40
Operator : JU
Sample : K6325-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT-3860

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

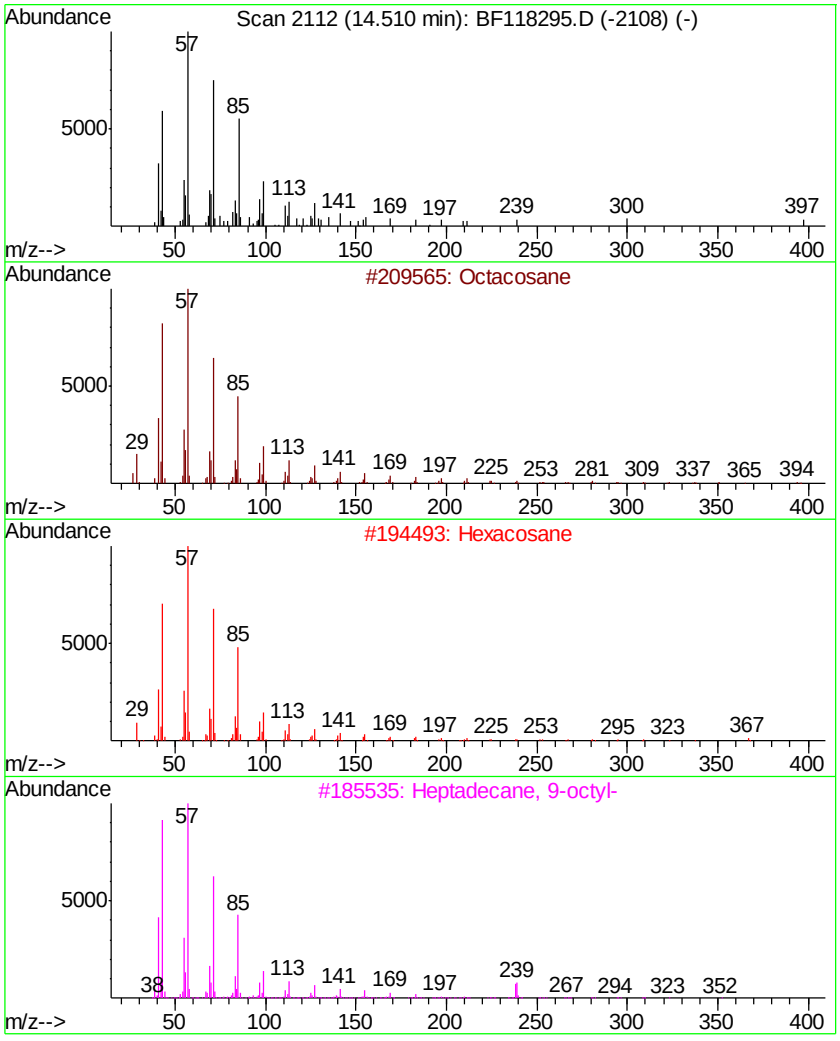
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

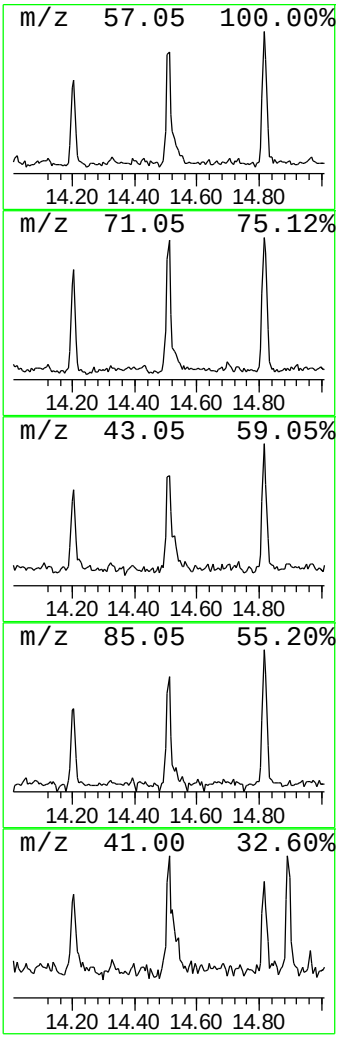
**********

Peak Number 6 Octacosane Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.51 | 2.72 ng | 109849 | Chrysene-d12 | 14.05 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 2 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |
| 3 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 90 |
| 4 | Tetracosane | 338 | C24H50 | 000646-31-1 | 87 |
| 5 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 87 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\
Data File : BF118295.D
Acq On : 19 Dec 2019 22:40
Operator : JU
Sample : K6325-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT-3860

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

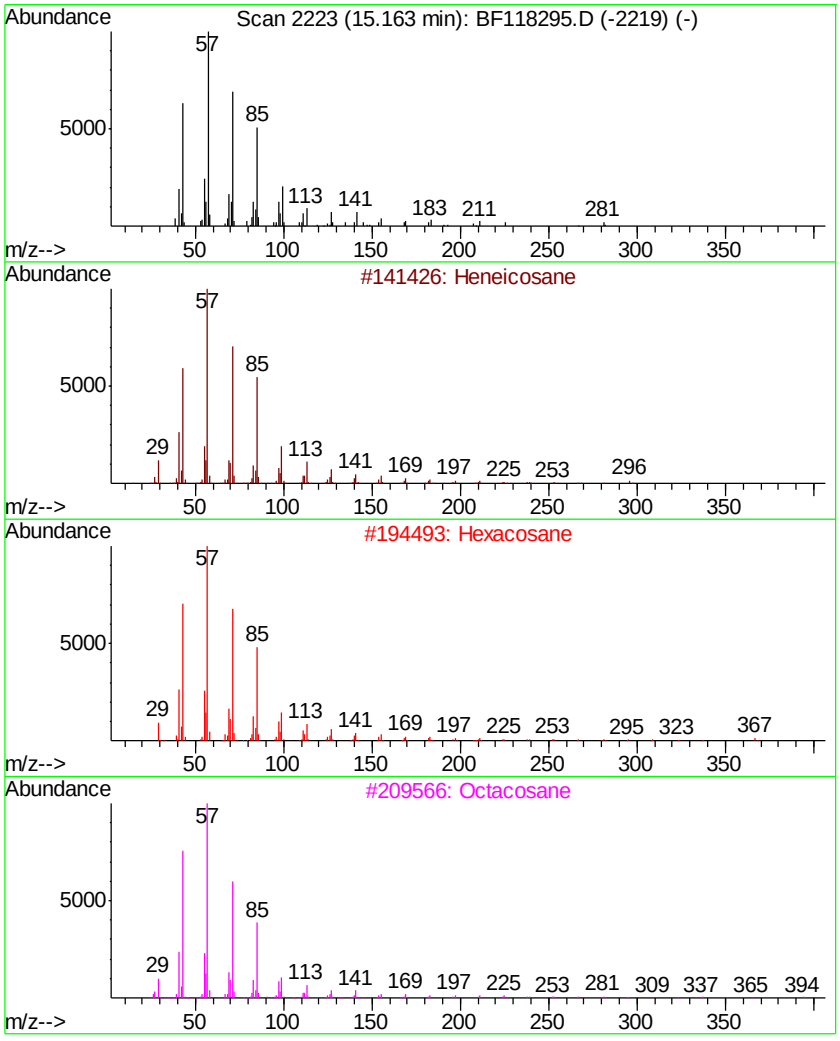
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

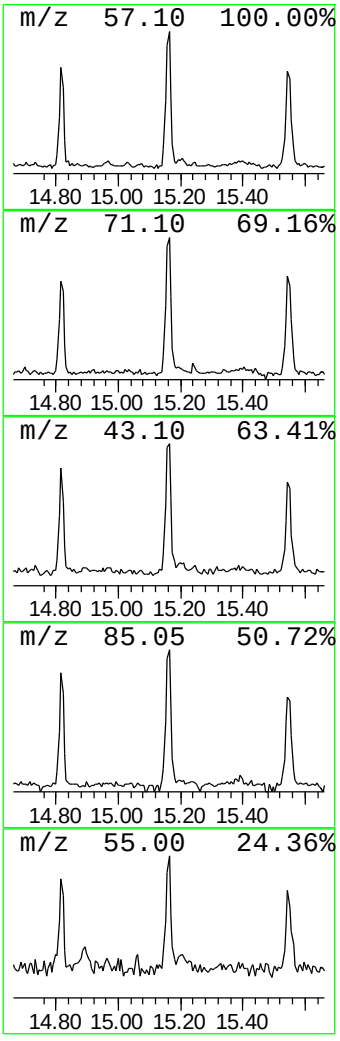
**********

Peak Number 7 Heneicosane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.16 | 2.80 ng | 110226 | Perylene-d12 | 15.54 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 2 | Hexacosane | 366 | C26H54 | 000630-01-3 | 91 |
| 3 | Octacosane | 394 | C28H58 | 000630-02-4 | 87 |
| 4 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 86 |
| 5 | Hexadecane | 226 | C16H34 | 000544-76-3 | 86 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\
Data File : BF118295.D
Acq On : 19 Dec 2019 22:40
Operator : JU
Sample : K6325-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT-3860

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

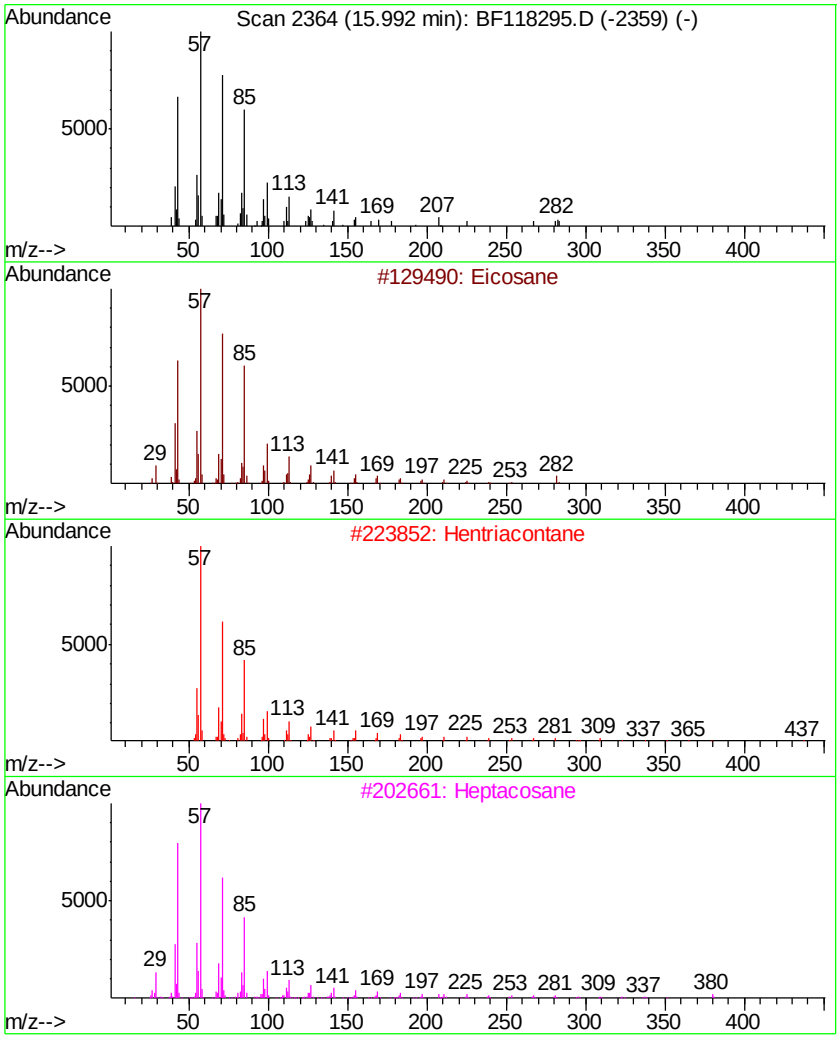
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

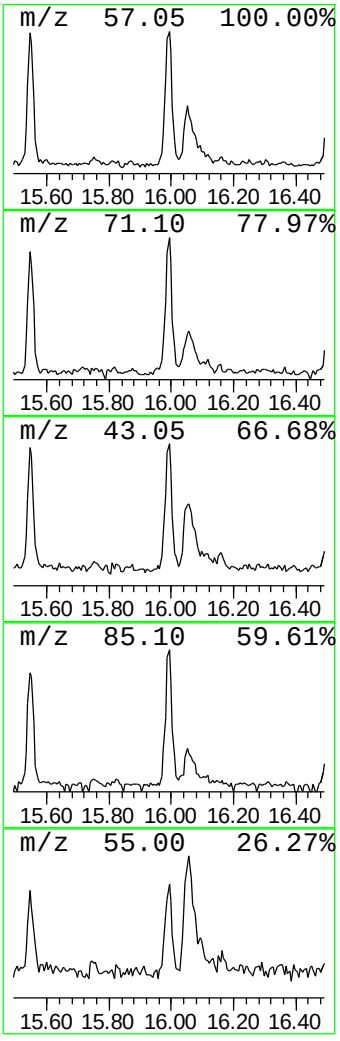
**********

Peak Number 8 Eicosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.99 | 2.89 ng | 113600 | Perylene-d12 | 15.54 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 95 |
| 2 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 91 |
| 3 | Heptacosane | 380 | C27H56 | 000593-49-7 | 90 |
| 4 | Eicosane, 7-hexyl- | 366 | C26H54 | 055333-99-8 | 90 |
| 5 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 90 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\
Data File : BF118295.D
Acq On : 19 Dec 2019 22:40
Operator : JU
Sample : K6325-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT-3860

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

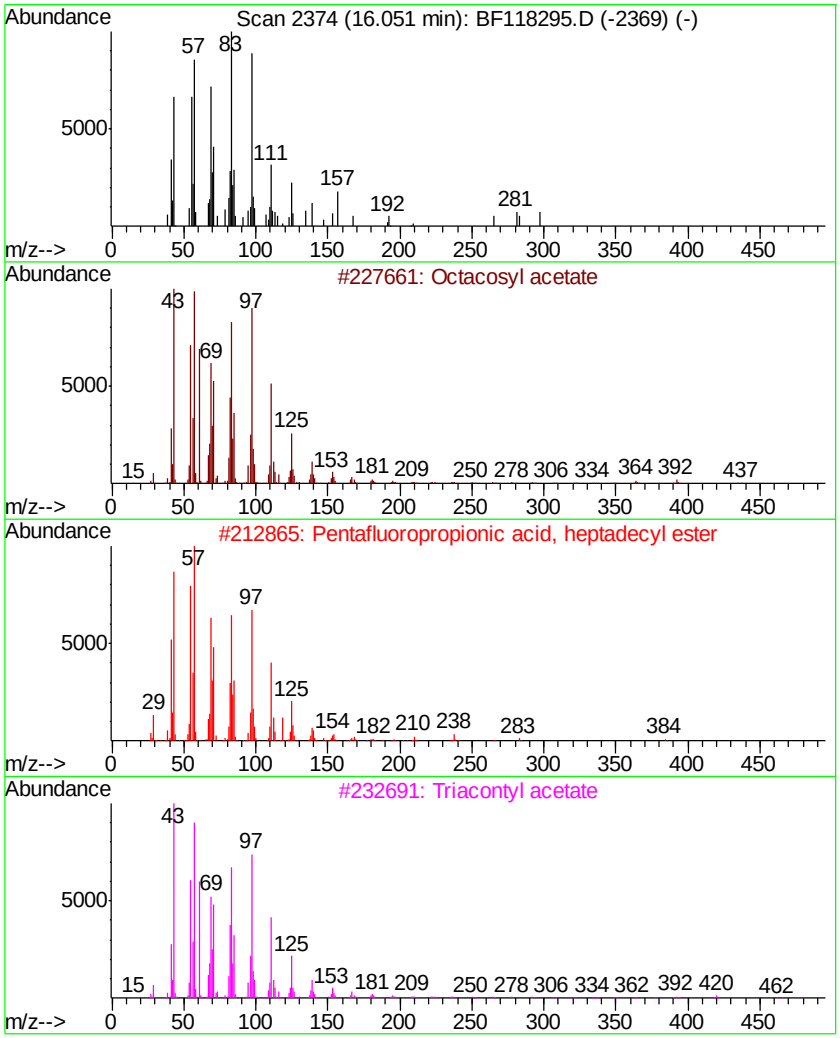
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

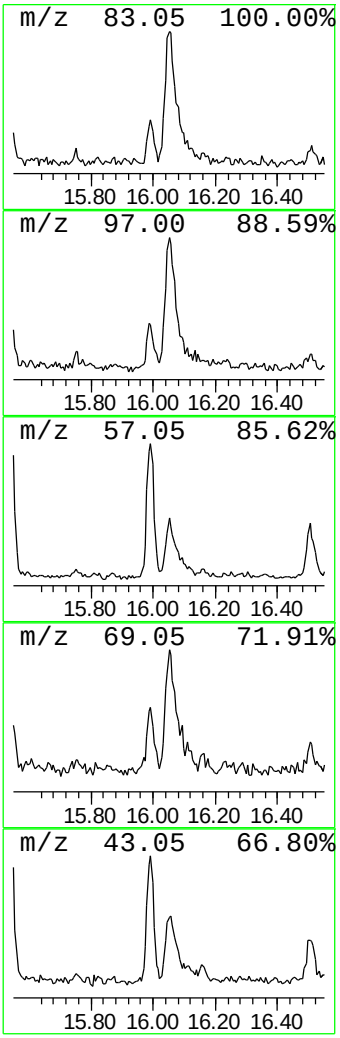
**********

Peak Number 9 Octacosyl acetate Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.05 | 3.68 ng | 144709 | Perylene-d12 | 15.54 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosyl acetate | 452 | C30H60O2 | 018206-97-8 | 64 |
| 2 | Pentafluoropropionic acid, hepta... | 402 | C20H35F5O2 | 959218-78-1 | 58 |
| 3 | Triacontyl acetate | 480 | C32H64O2 | 041755-58-2 | 58 |
| 4 | Pentafluoropropionic acid, octad... | 416 | C21H37F5O2 | 959261-25-7 | 58 |
| 5 | Heptafluorobutyric acid, n-octad... | 466 | C22H37F7O2 | 000400-57-7 | 58 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121919\
Data File : BF118295.D
Acq On : 19 Dec 2019 22:40
Operator : JU
Sample : K6325-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT-3860

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 5.06 | 13.2 | ng | 390064 | 1 | 6.86 | 591434 | 20.0 |
| unknown6.63 | 6.63 | 83.0 | ng | 2454110 | 1 | 6.86 | 591434 | 20.0 |
| n-Hexadecanoic acid | 11.92 | 6.2 | ng | 287696 | 4 | 11.40 | 929096 | 20.0 |
| Trifluoroacetoxy ... | 13.88 | 11.4 | ng | 459354 | 5 | 14.05 | 808899 | 20.0 |
| Octacosane | 14.51 | 2.7 | ng | 109849 | 5 | 14.05 | 808899 | 20.0 |
| Heneicosane | 15.16 | 2.8 | ng | 110226 | 6 | 15.54 | 787481 | 20.0 |
| Eicosane | 15.99 | 2.9 | ng | 113600 | 6 | 15.54 | 787481 | 20.0 |
| Octacosyl acetate | 16.05 | 3.7 | ng | 144709 | 6 | 15.54 | 787481 | 20.0 |