LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100918\
Data File : BF109721.D
Acq On : 10 Oct 2018 3:28
Operator : JU/SJ
Sample : J5326-21
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FL-PIT-6

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-BF100818.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 | 4.904 | 476 | 479 | 490 | rBV | 50469 | 76771 | 3.36% | 0.428% |
| 2 | 5.316 | 545 | 549 | 570 | rBV | 1495176 | 1933445 | 84.72% | 10.776% |
| 3 | 6.346 | 720 | 724 | 741 | rBV | 1575406 | 2153147 | 94.35% | 12.000% |
| 4 | 6.469 | 741 | 745 | 770 | rVB | 2057393 | 2282051 | 100.00% | 12.719% |
| 5 | 6.698 | 781 | 784 | 794 | rBV | 279413 | 390545 | 17.11% | 2.177% |
| 6 | 6.851 | 806 | 810 | 850 | rVB | 1633482 | 1699557 | 74.47% | 9.472% |
| 7 | 7.257 | 876 | 879 | 900 | rBV | 923127 | 1336557 | 58.57% | 7.449% |
| 8 | 7.975 | 998 | 1001 | 1025 | rBV | 373580 | 489091 | 21.43% | 2.726% |
| 9 | 9.051 | 1180 | 1184 | 1210 | rBV | 1928553 | 2098599 | 91.96% | 11.696% |
| 10 | 9.445 | 1247 | 1251 | 1264 | rBV | 122595 | 145088 | 6.36% | 0.809% |
| 11 | 9.722 | 1294 | 1298 | 1317 | rBV | 440015 | 467420 | 20.48% | 2.605% |
| 12 | 10.510 | 1428 | 1432 | 1451 | rBV | 848668 | 1085232 | 47.56% | 6.048% |
| 13 | 11.204 | 1546 | 1550 | 1567 | rBV | 279358 | 410548 | 17.99% | 2.288% |
| 14 | 12.780 | 1814 | 1818 | 1838 | rBV | 1823351 | 1739497 | 76.23% | 9.695% |
| 15 | 13.686 | 1968 | 1972 | 1990 | rBV3 | 43816 | 115145 | 5.05% | 0.642% |
| 16 | 13.827 | 1992 | 1996 | 2009 | rVB | 475571 | 526197 | 23.06% | 2.933% |
| 17 | 13.998 | 2021 | 2025 | 2029 | rBV | 29151 | 24079 | 1.06% | 0.134% |
| 18 | 14.298 | 2071 | 2076 | 2079 | rBV | 37355 | 39005 | 1.71% | 0.217% |
| 19 | 14.592 | 2123 | 2126 | 2130 | rVB | 46349 | 44411 | 1.95% | 0.248% |
| 20 | 14.904 | 2175 | 2179 | 2183 | rBV | 67023 | 69860 | 3.06% | 0.389% |
| 21 | 15.221 | 2229 | 2233 | 2246 | rBV | 276477 | 495409 | 21.71% | 2.761% |
| 22 | 15.645 | 2300 | 2305 | 2314 | rVB | 77555 | 111463 | 4.88% | 0.621% |
| 23 | 16.098 | 2376 | 2382 | 2395 | rVB2 | 53554 | 99595 | 4.36% | 0.555% |
| 24 | 16.633 | 2468 | 2473 | 2480 | rVB3 | 31935 | 61217 | 2.68% | 0.341% |
| 25 | 17.262 | 2574 | 2580 | 2590 | rVB3 | 19225 | 48330 | 2.12% | 0.269% |

Sum of corrected areas: 17942259

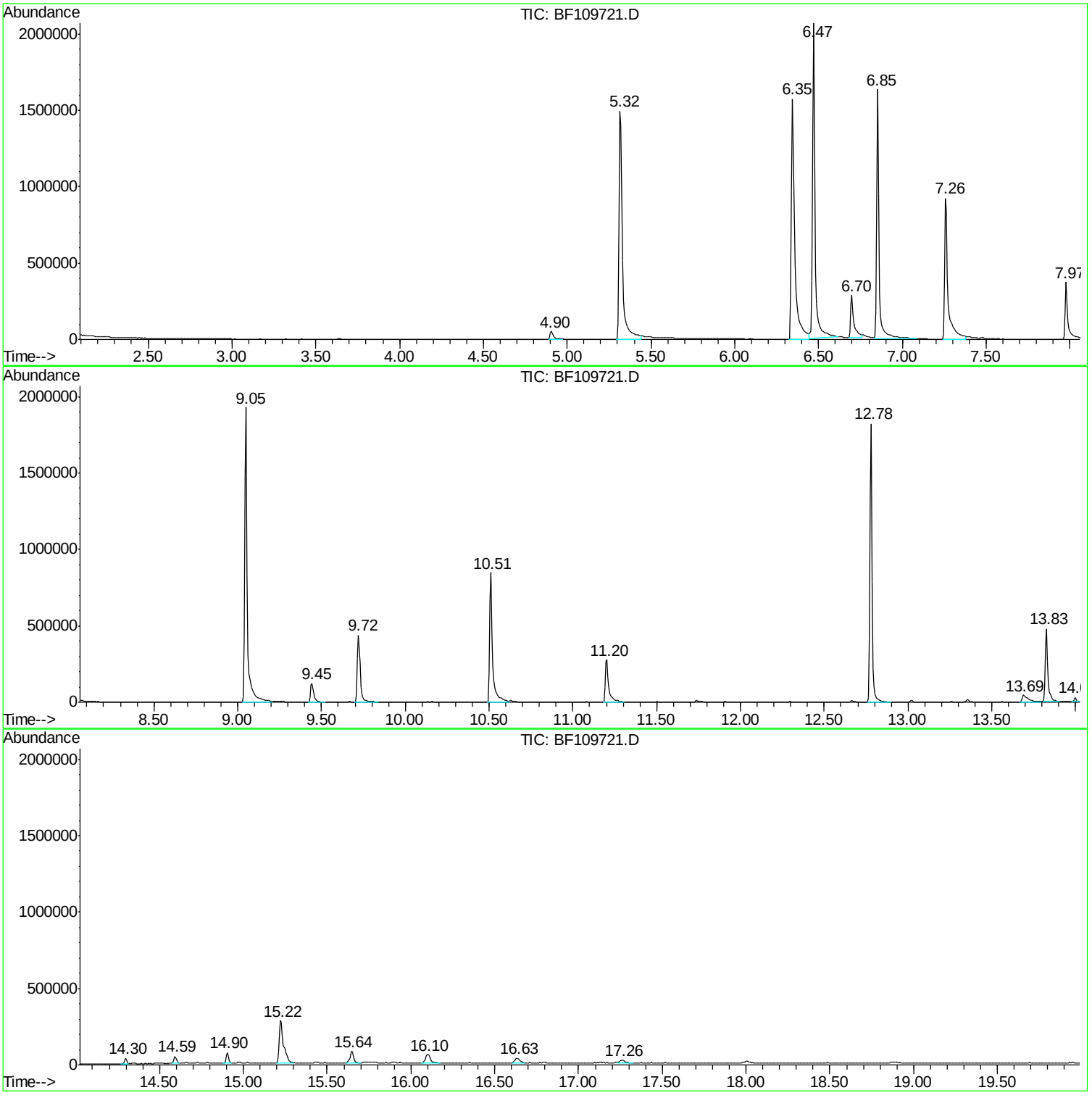
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100918\
Data File : BF109721.D
Acq On : 10 Oct 2018 3:28
Operator : JU/SJ
Sample : J5326-21
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FL-PIT-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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\BF100918\
Data File : BF109721.D
Acq On : 10 Oct 2018 3:28
Operator : JU/SJ
Sample : J5326-21
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FL-PIT-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

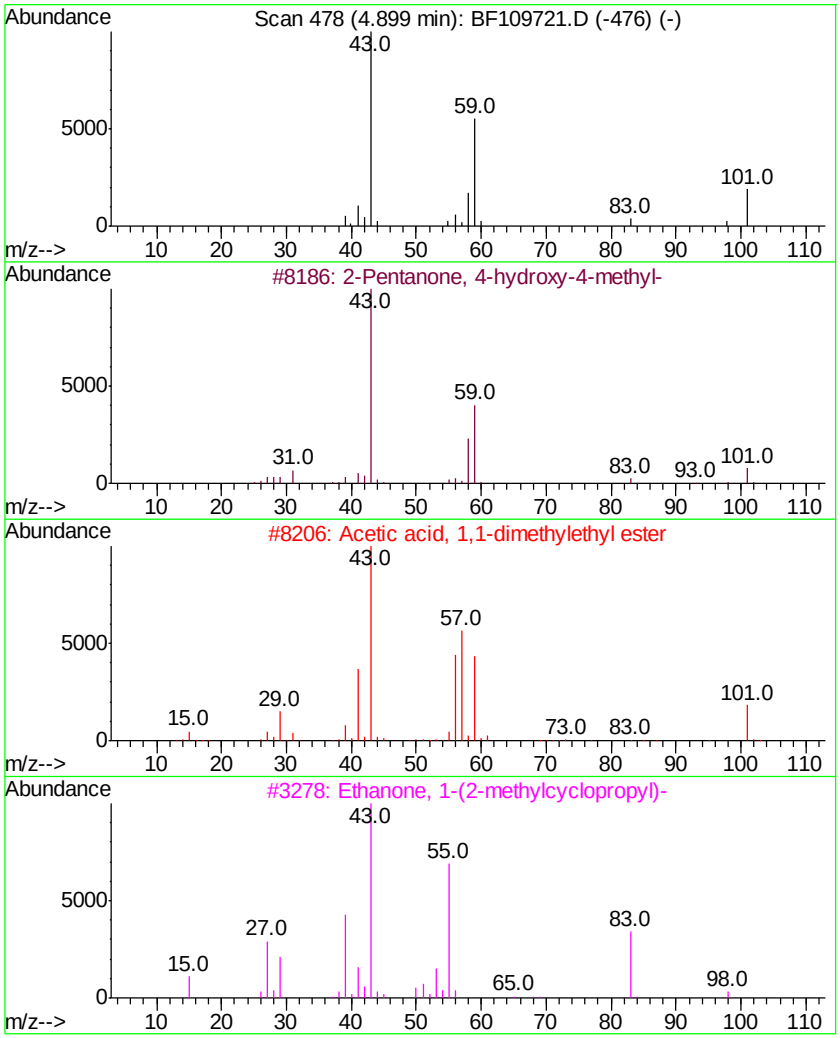
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

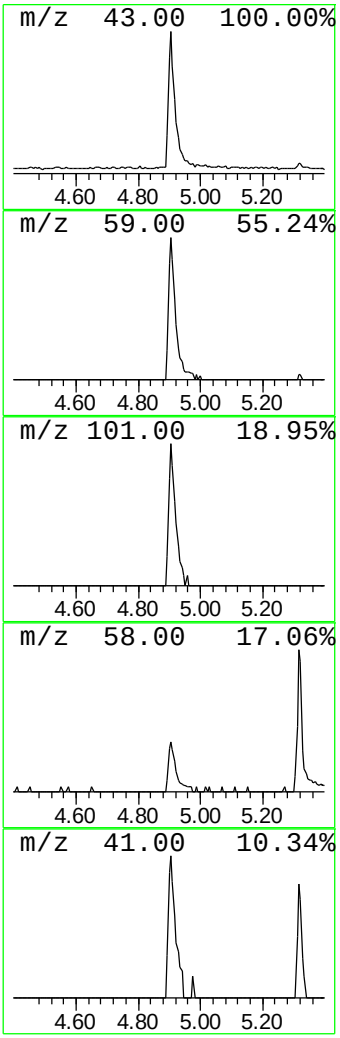
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.90 | 3.93 ng | 76771 | 1,4-Dichlorobenzene-d4 | 6.70 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 42 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39 |
| 3 | Ethanone, 1-(2-methylcyclopropyl)- | 98 | C6H10O | 000930-56-3 | 9 |
| 4 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |
| 5 | Acetone | 58 | C3H6O | 000067-64-1 | 9 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100918\
Data File : BF109721.D
Acq On : 10 Oct 2018 3:28
Operator : JU/SJ
Sample : J5326-21
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FL-PIT-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

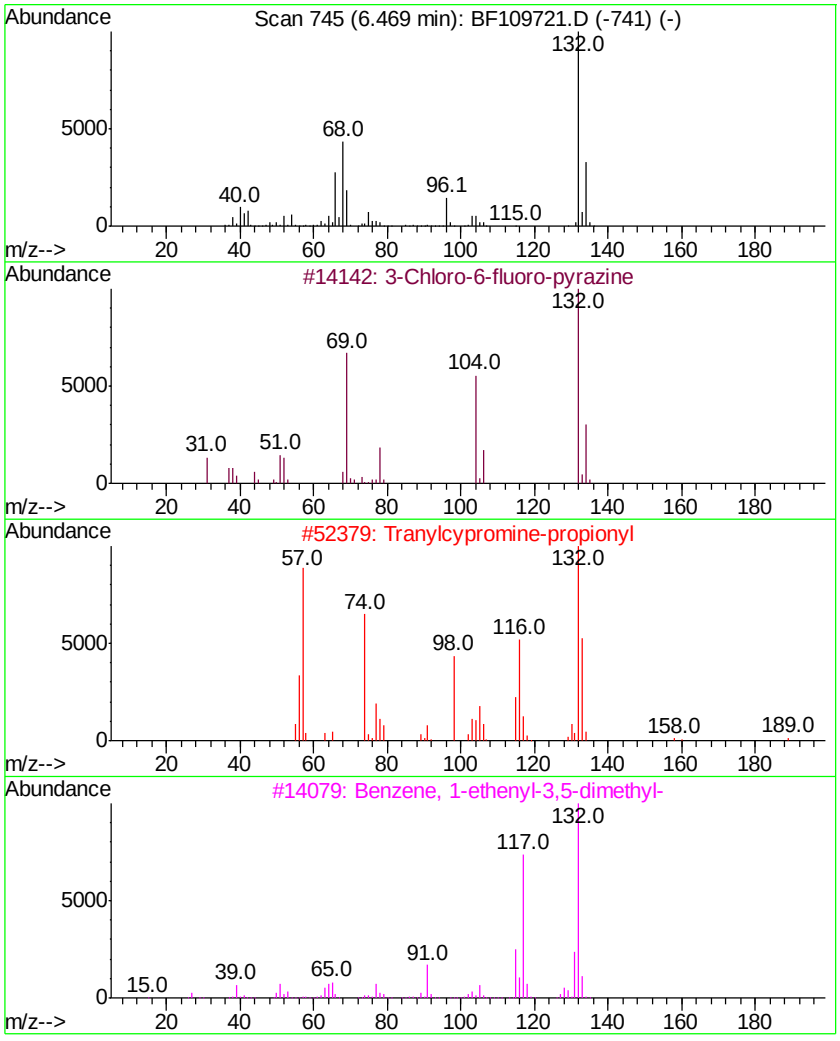
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

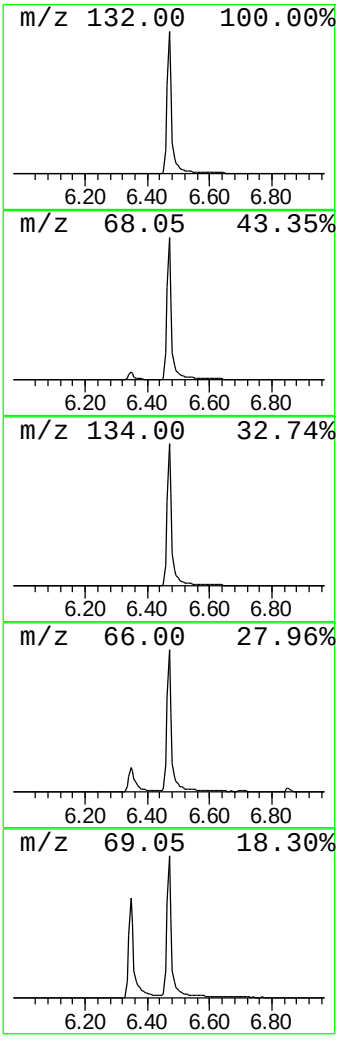
**********

Peak Number 2 unknown6.47 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.47 | 116.87 ng | 2282050 | 1,4-Dichlorobenzene-d4 | 6.70 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 3 | Benzene, 1-ethenyl-3,5-dimethyl- | 132 | C10H12 | 005379-20-4 | 9 |
| 4 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 9 |
| 5 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100918\
Data File : BF109721.D
Acq On : 10 Oct 2018 3:28
Operator : JU/SJ
Sample : J5326-21
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FL-PIT-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

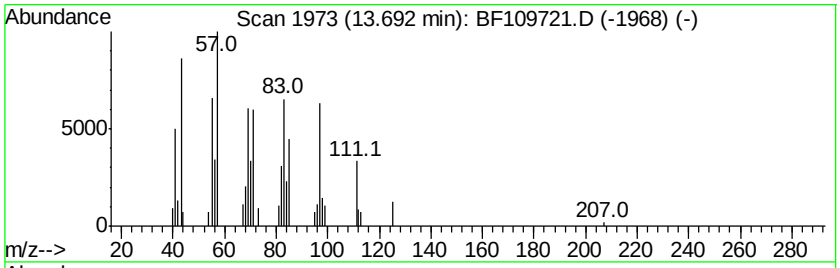
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

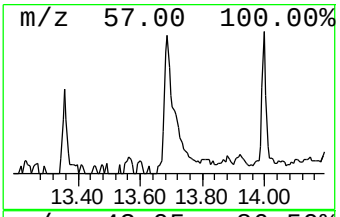
**********

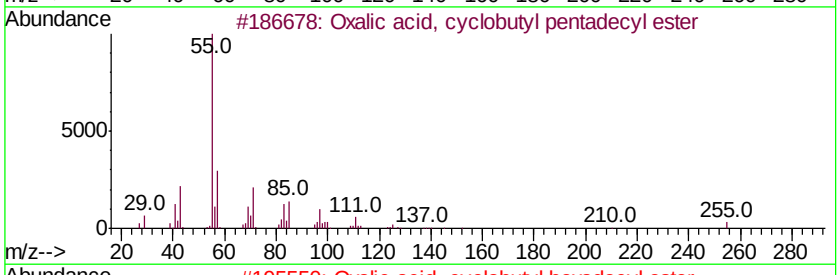
Peak Number 4 Oxalic acid, cyclobutyl pen... Concentration Rank 4

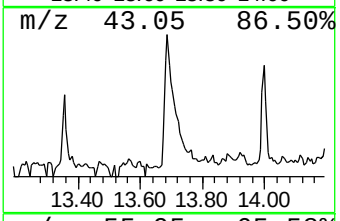
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.69 | 4.38 ng | 115145 | Chrysene-d12 | 13.83 |

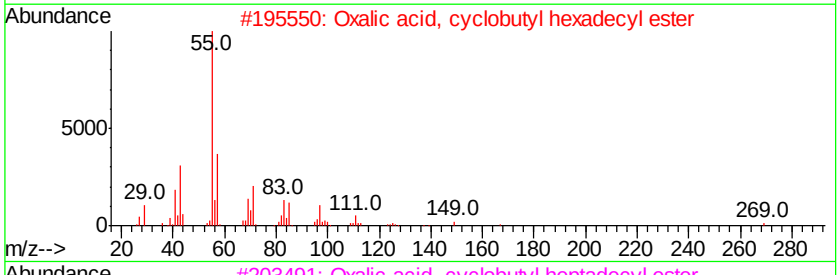
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Oxalic acid, cyclobutyl pentadec... | 354 | C21H38O4 | 1000309-70-5 | 90 |
| 2 | Oxalic acid, cyclobutyl hexadecy... | 368 | C22H40O4 | 1000309-70-6 | 90 |
| 3 | Oxalic acid, cyclobutyl heptadec... | 382 | C23H42O4 | 1000309-70-7 | 80 |
| 4 | 1-Dodecanol, 2-octyl- | 298 | C20H42O | 005333-42-6 | 68 |
| 5 | 3-Eicosene, (E)- | 280 | C20H40 | 074685-33-9 | 64 |

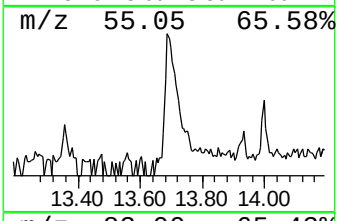


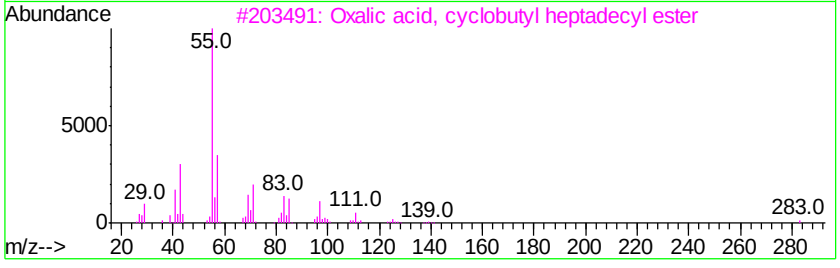



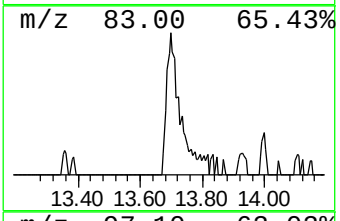



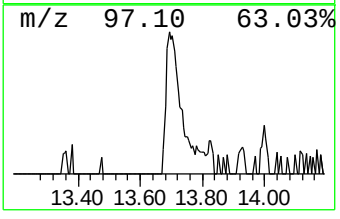



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100918\
Data File : BF109721.D
Acq On : 10 Oct 2018 3:28
Operator : JU/SJ
Sample : J5326-21
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FL-PIT-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

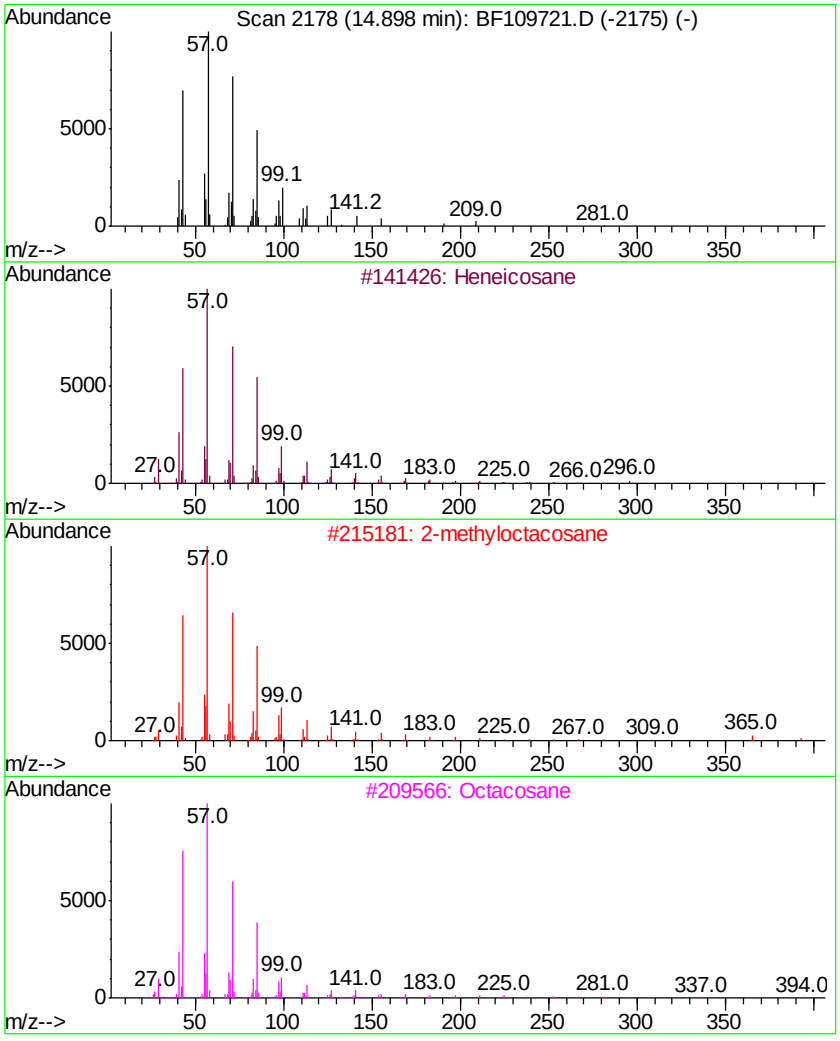
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

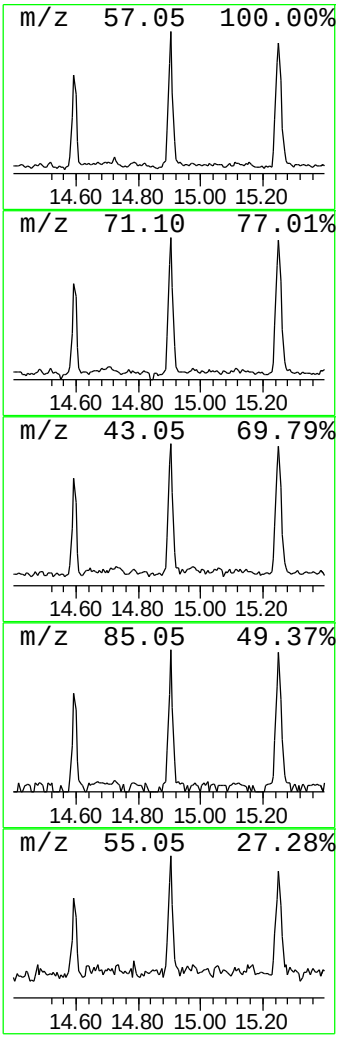
**********

Peak Number 5 Heneicosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.90 | 2.82 ng | 69860 | Perylene-d12 | 15.22 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 2 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 91 |
| 3 | Octacosane | 394 | C28H58 | 000630-02-4 | 87 |
| 4 | Heptadecane | 240 | C17H36 | 000629-78-7 | 87 |
| 5 | Hexacosane | 366 | C26H54 | 000630-01-3 | 87 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100918\
Data File : BF109721.D
Acq On : 10 Oct 2018 3:28
Operator : JU/SJ
Sample : J5326-21
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FL-PIT-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

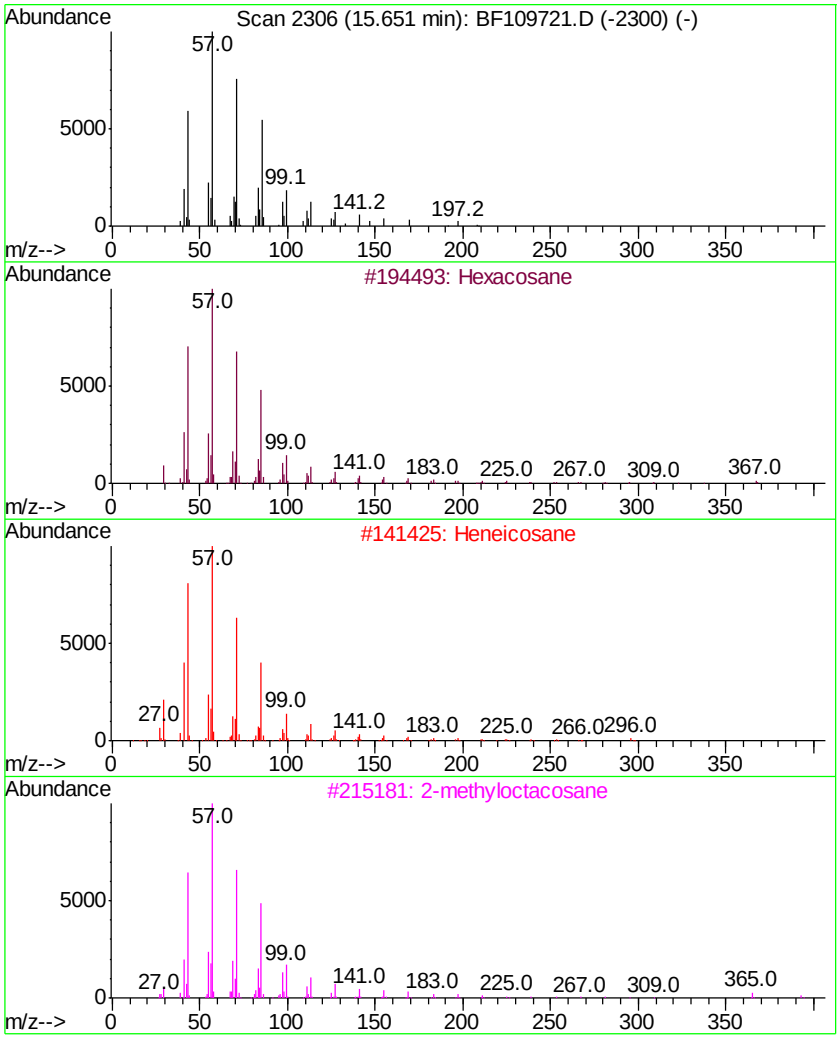
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

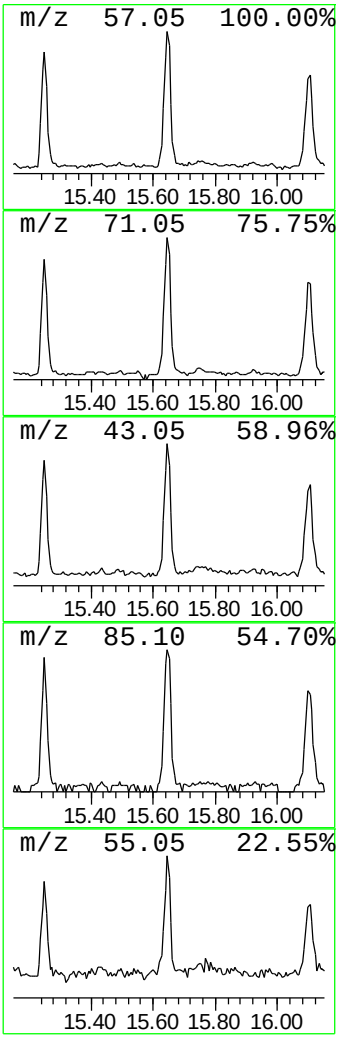
**********

Peak Number 6 Hexacosane Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.65 | 4.50 ng | 111463 | Perylene-d12 | 15.22 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexacosane | 366 | C26H54 | 000630-01-3 | 91 |
| 2 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 3 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 91 |
| 4 | Heptacosane | 380 | C27H56 | 000593-49-7 | 91 |
| 5 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 90 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100918\
Data File : BF109721.D
Acq On : 10 Oct 2018 3:28
Operator : JU/SJ
Sample : J5326-21
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FL-PIT-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

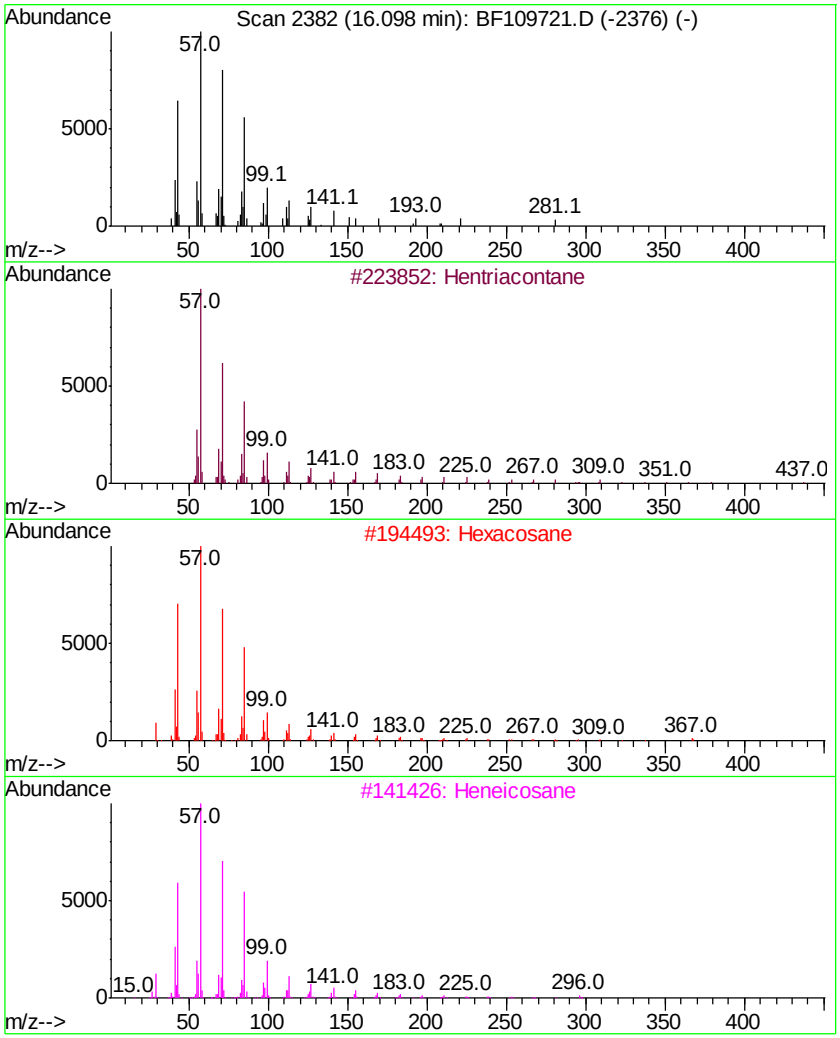
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

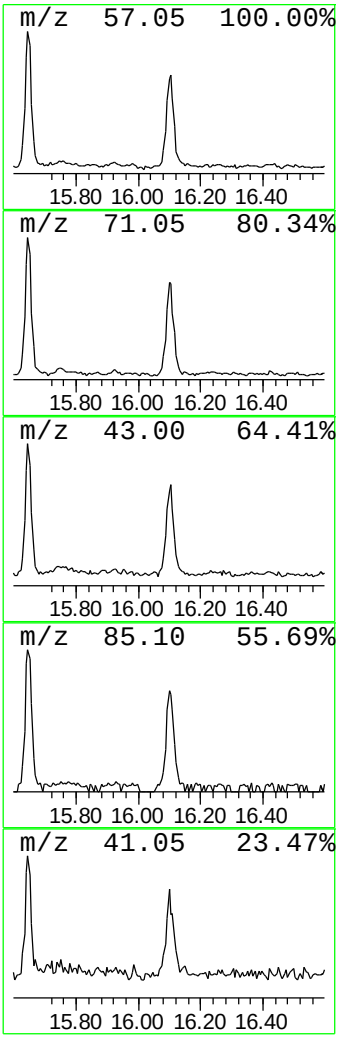
**********

Peak Number 7 Hentriacontane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.10 | 4.02 ng | 99595 | Perylene-d12 | 15.22 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 91 |
| 2 | Hexacosane | 366 | C26H54 | 000630-01-3 | 91 |
| 3 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 4 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 5 | Heptacosane | 380 | C27H56 | 000593-49-7 | 91 |



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Sample : J5326-21
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FL-PIT-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

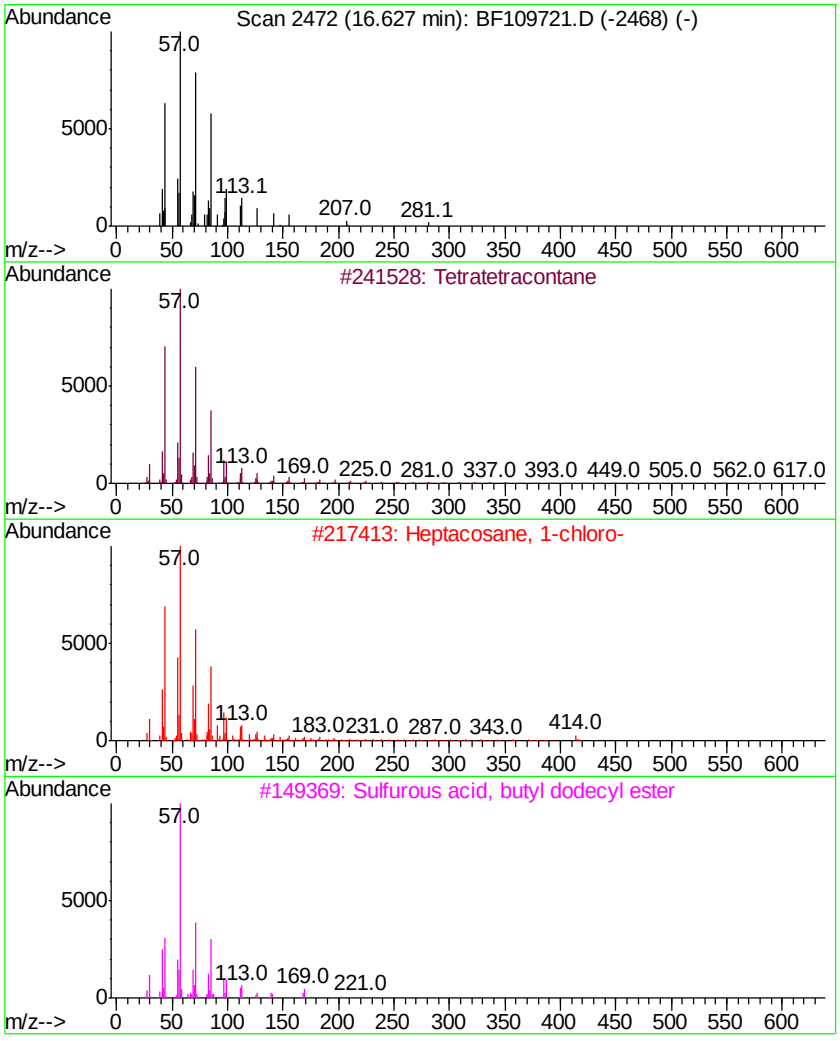
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

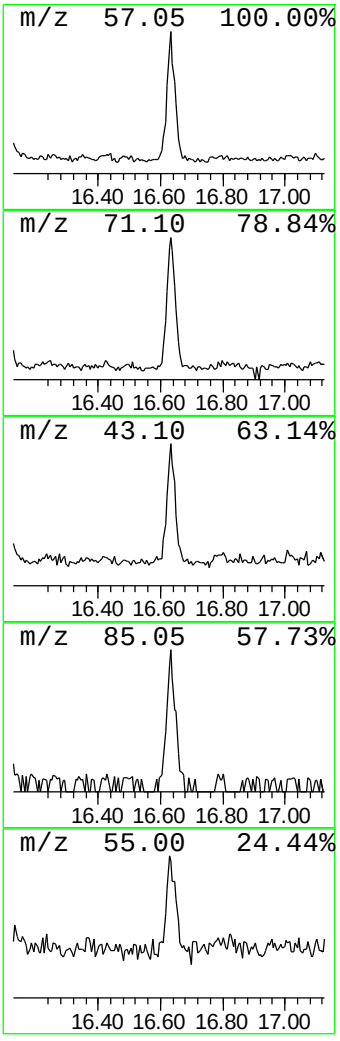
**********

Peak Number 8 Tetratetracontane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.63 | 2.47 ng | 61217 | Perylene-d12 | 15.22 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 91 |
| 2 | Heptacosane, 1-chloro- | 414 | C27H55Cl | 062016-79-9 | 90 |
| 3 | Sulfurous acid, butyl dodecyl ester | 306 | C16H34O3S | 1000309-17-9 | 90 |
| 4 | Heptacosane | 380 | C27H56 | 000593-49-7 | 90 |
| 5 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100918\
Data File : BF109721.D
Acq On : 10 Oct 2018 3:28
Operator : JU/SJ
Sample : J5326-21
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FL-PIT-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100818.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... | 4.90 | 3.9 | ng | 76771 | 1 | 6.70 | 390545 | 20.0 |
| unknown6.47 | 6.47 | 116.9 | ng | 2282050 | 1 | 6.70 | 390545 | 20.0 |
| Oxalic acid, cycl... | 13.69 | 4.4 | ng | 115145 | 5 | 13.83 | 526197 | 20.0 |
| Heneicosane | 14.90 | 2.8 | ng | 69860 | 6 | 15.22 | 495409 | 20.0 |
| Hexacosane | 15.65 | 4.5 | ng | 111463 | 6 | 15.22 | 495409 | 20.0 |
| Hentriacontane | 16.10 | 4.0 | ng | 99595 | 6 | 15.22 | 495409 | 20.0 |
| Tetratetracontane | 16.63 | 2.5 | ng | 61217 | 6 | 15.22 | 495409 | 20.0 |