LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122018\
Data File : BF111645.D
Acq On : 20 Dec 2018 18:15
Operator : JU/SJ
Sample : J6353-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS003-0002-01

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-BF121918.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 | 2.222 | 20 | 23 | 30 | rVB | 65407 | 91687 | 2.50% | 0.294% |
| 2 | 5.116 | 509 | 515 | 522 | rVB | 174836 | 207865 | 5.67% | 0.666% |
| 3 | 5.522 | 579 | 584 | 587 | rBV | 3471158 | 3157389 | 86.06% | 10.115% |
| 4 | 6.522 | 748 | 754 | 760 | rBV | 3520204 | 3668909 | 100.00% | 11.754% |
| 5 | 6.663 | 774 | 778 | 782 | rBV | 3480420 | 3319876 | 90.49% | 10.636% |
| 6 | 6.898 | 814 | 818 | 821 | rBV | 1379640 | 1230312 | 33.53% | 3.942% |
| 7 | 7.051 | 840 | 844 | 848 | rVB | 2446128 | 1997838 | 54.45% | 6.400% |
| 8 | 7.451 | 907 | 912 | 915 | rBV | 2264304 | 2002967 | 54.59% | 6.417% |
| 9 | 8.175 | 1031 | 1035 | 1039 | rBV | 1788997 | 1564628 | 42.65% | 5.013% |
| 10 | 9.251 | 1213 | 1218 | 1221 | rBV | 2867992 | 2317093 | 63.15% | 7.423% |
| 11 | 9.639 | 1280 | 1284 | 1287 | rBV | 399614 | 292775 | 7.98% | 0.938% |
| 12 | 9.933 | 1328 | 1334 | 1337 | rBV | 1884903 | 1712477 | 46.68% | 5.486% |
| 13 | 10.339 | 1398 | 1403 | 1406 | rBV2 | 26033 | 44121 | 1.20% | 0.141% |
| 14 | 10.716 | 1462 | 1467 | 1470 | rBV | 2098526 | 1939933 | 52.87% | 6.215% |
| 15 | 11.274 | 1559 | 1562 | 1566 | rBV3 | 59373 | 58746 | 1.60% | 0.188% |
| 16 | 11.410 | 1582 | 1585 | 1589 | rBV | 1594428 | 1482095 | 40.40% | 4.748% |
| 17 | 11.810 | 1650 | 1653 | 1657 | rBV | 112484 | 91289 | 2.49% | 0.292% |
| 18 | 11.939 | 1671 | 1675 | 1679 | rBV | 449992 | 403072 | 10.99% | 1.291% |
| 19 | 12.721 | 1805 | 1808 | 1816 | rBV | 228082 | 242931 | 6.62% | 0.778% |
| 20 | 12.868 | 1830 | 1833 | 1836 | rBV | 122465 | 110325 | 3.01% | 0.353% |
| 21 | 12.992 | 1850 | 1854 | 1858 | rBV | 2126212 | 1853057 | 50.51% | 5.937% |
| 22 | 13.468 | 1933 | 1935 | 1937 | rBV | 77582 | 56650 | 1.54% | 0.181% |
| 23 | 13.892 | 2003 | 2007 | 2013 | rBV | 479028 | 495403 | 13.50% | 1.587% |
| 24 | 14.045 | 2028 | 2033 | 2037 | rBV | 1434469 | 1475697 | 40.22% | 4.728% |
| 25 | 15.527 | 2280 | 2285 | 2290 | rVB | 1020663 | 1280288 | 34.90% | 4.102% |
| 26 | 16.062 | 2373 | 2376 | 2384 | rBV5 | 60280 | 116762 | 3.18% | 0.374% |

Sum of corrected areas: 31214185

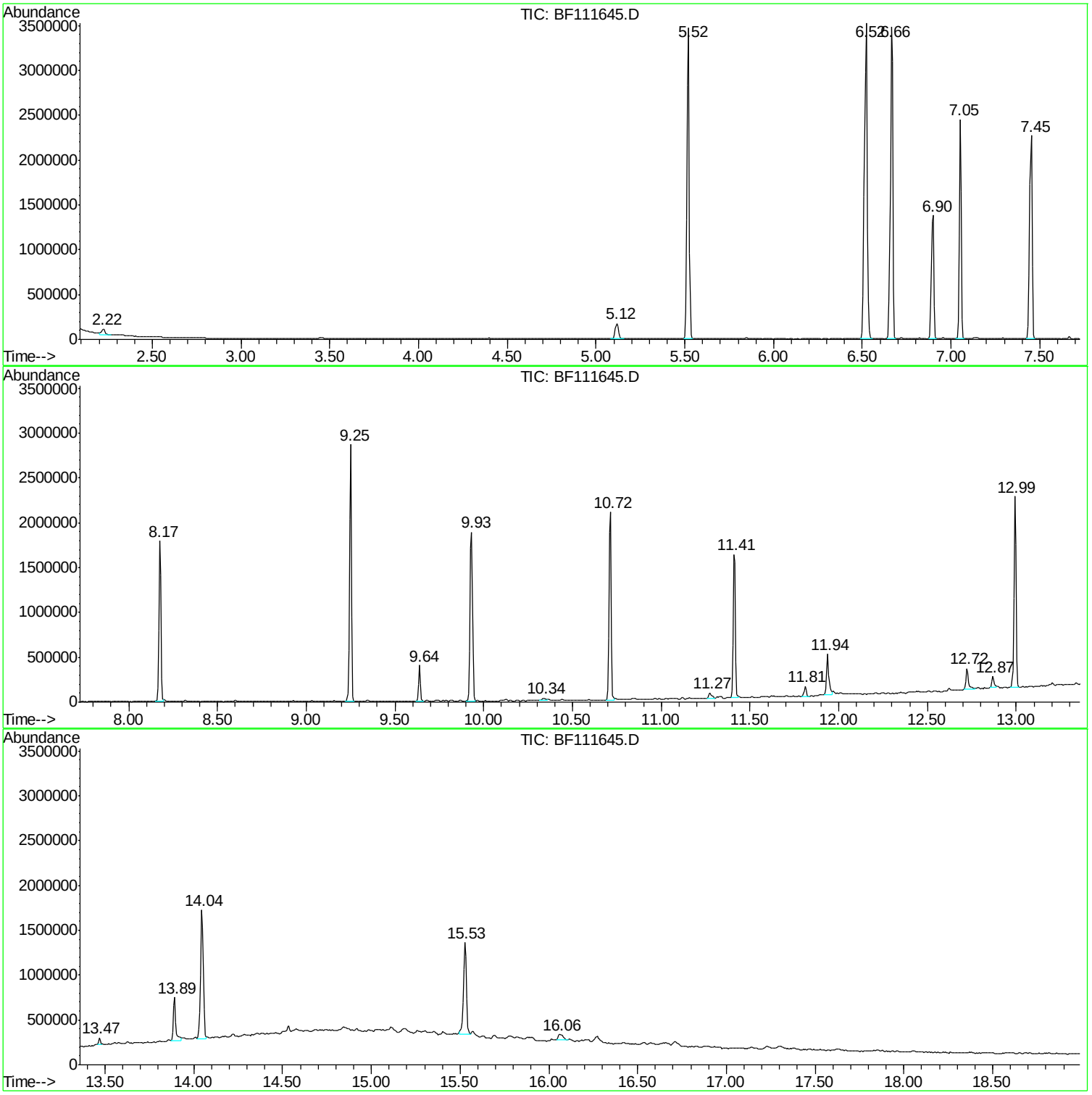
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122018\
Data File : BF111645.D
Acq On : 20 Dec 2018 18:15
Operator : JU/SJ
Sample : J6353-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS003-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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\BF122018\
Data File : BF111645.D
Acq On : 20 Dec 2018 18:15
Operator : JU/SJ
Sample : J6353-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS003-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

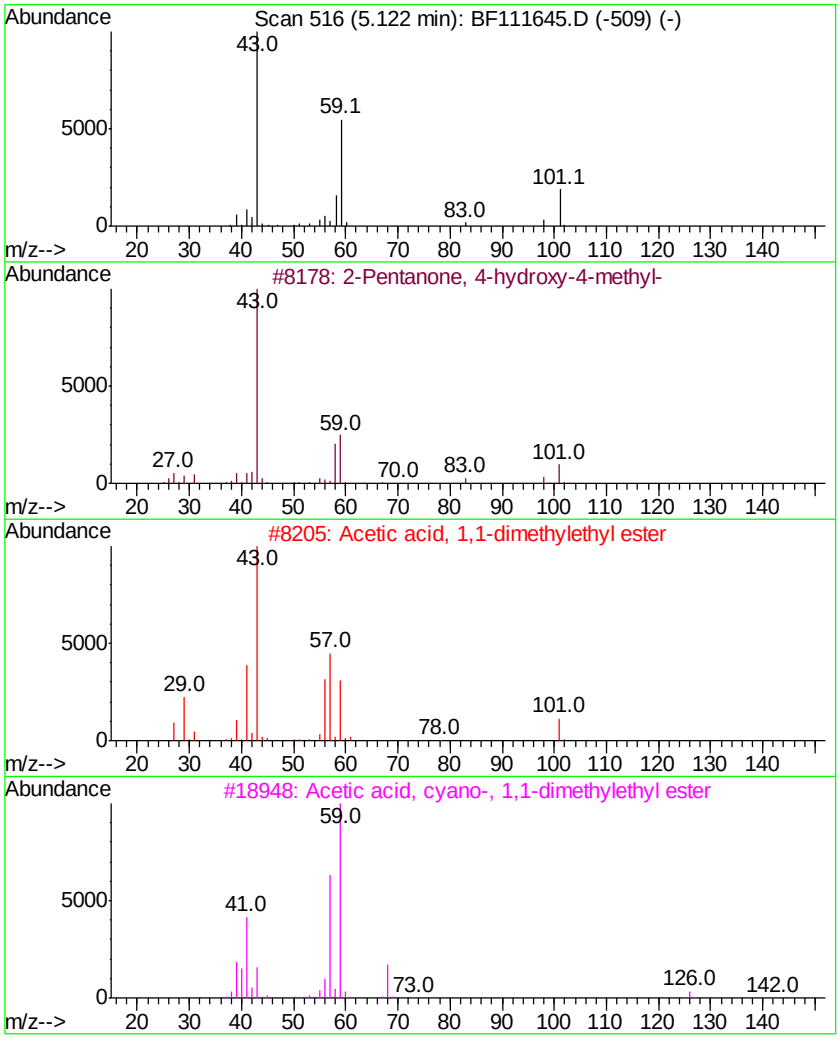
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

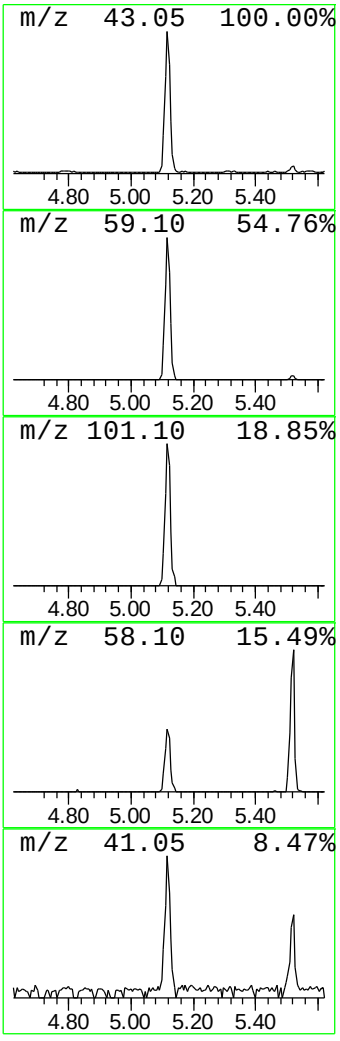
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.12 | 3.38 ng | 207865 | 1,4-Dichlorobenzene-d4 | 6.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 45 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 32 |
| 3 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |
| 4 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 10 |
| 5 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122018\
Data File : BF111645.D
Acq On : 20 Dec 2018 18:15
Operator : JU/SJ
Sample : J6353-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS003-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

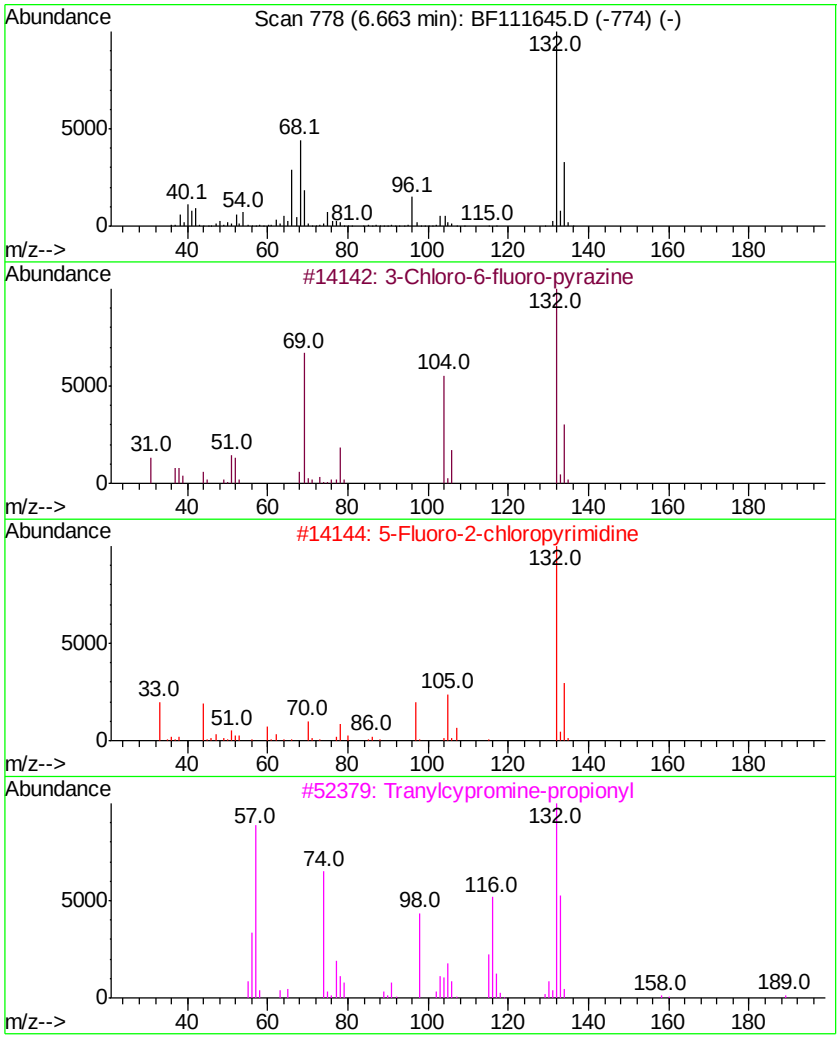
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

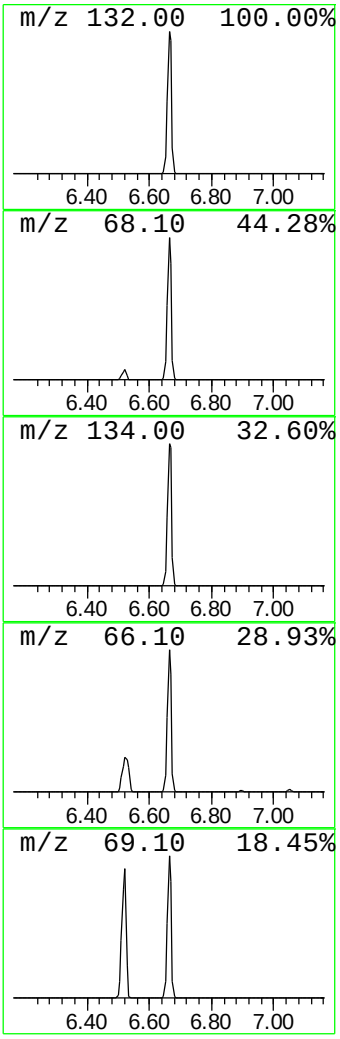
**********

Peak Number 2 unknown6.66 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.66 | 53.97 ng | 3319880 | 1,4-Dichlorobenzene-d4 | 6.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 12 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | 1,3,5-Trifluorobenzene | 132 | C6H3F3 | 000372-38-3 | 9 |
| 5 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 9 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122018\
Data File : BF111645.D
Acq On : 20 Dec 2018 18:15
Operator : JU/SJ
Sample : J6353-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS003-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

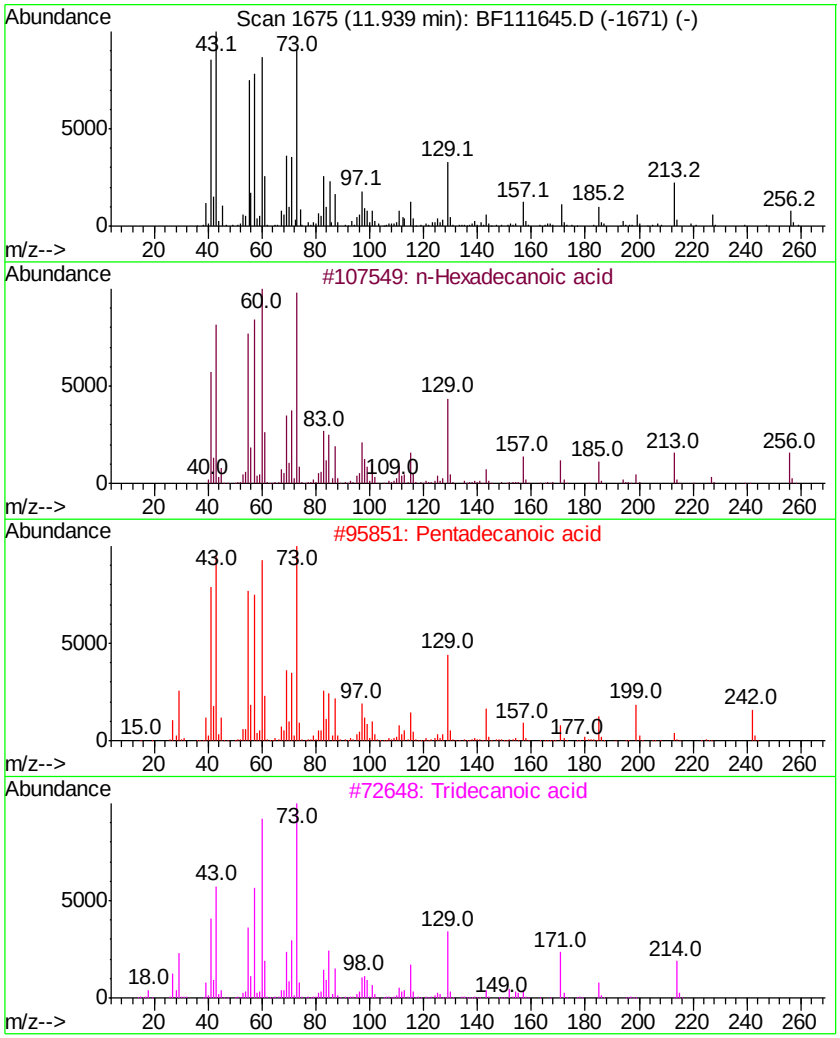
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

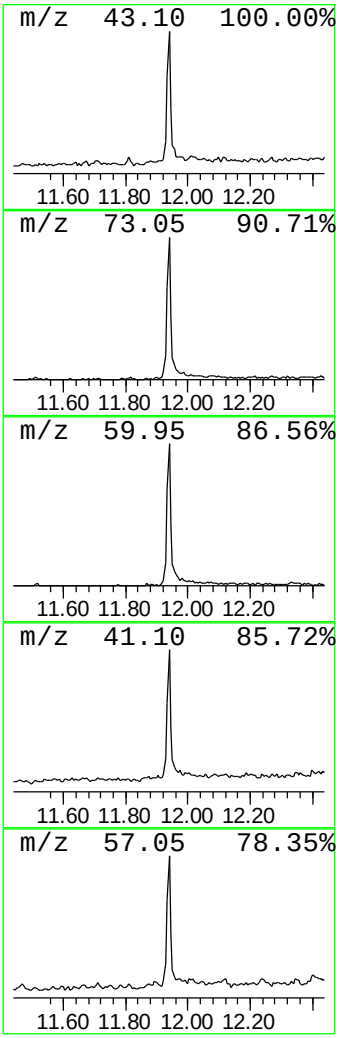
**********

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.94 | 5.44 ng | 403072 | Phenanthrene-d10 | 11.41 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 93 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 87 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 81 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 76 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 60 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122018\
Data File : BF111645.D
Acq On : 20 Dec 2018 18:15
Operator : JU/SJ
Sample : J6353-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS003-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

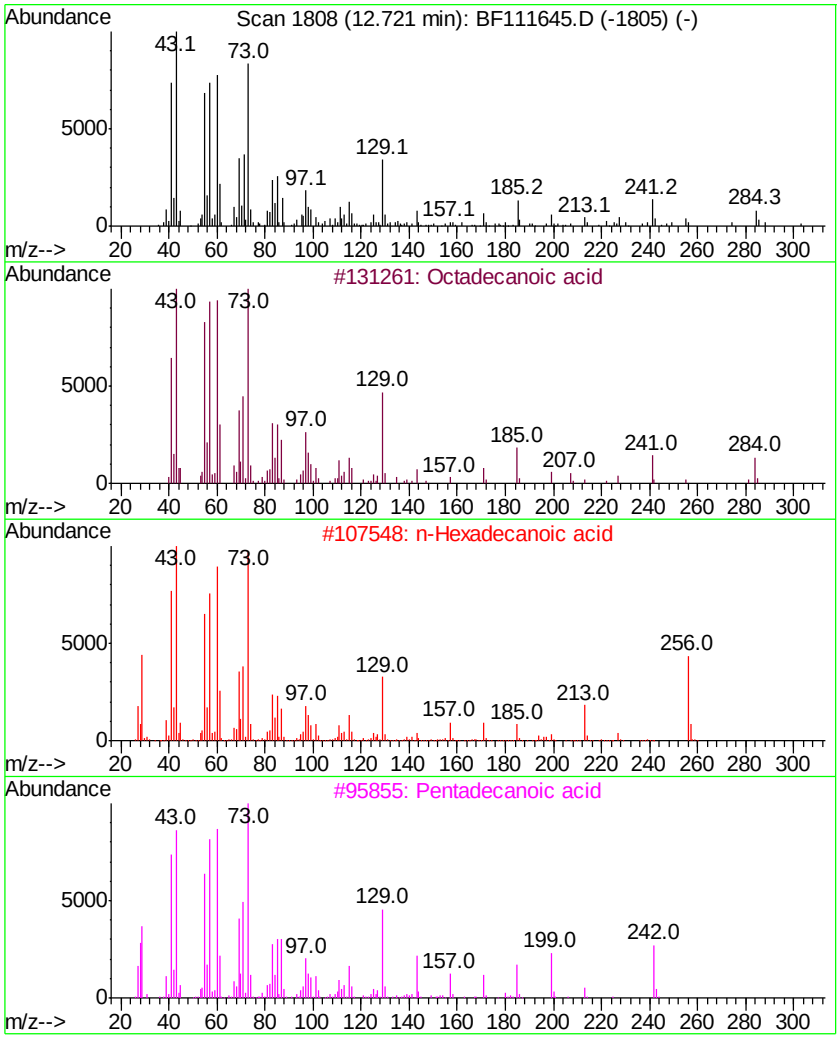
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

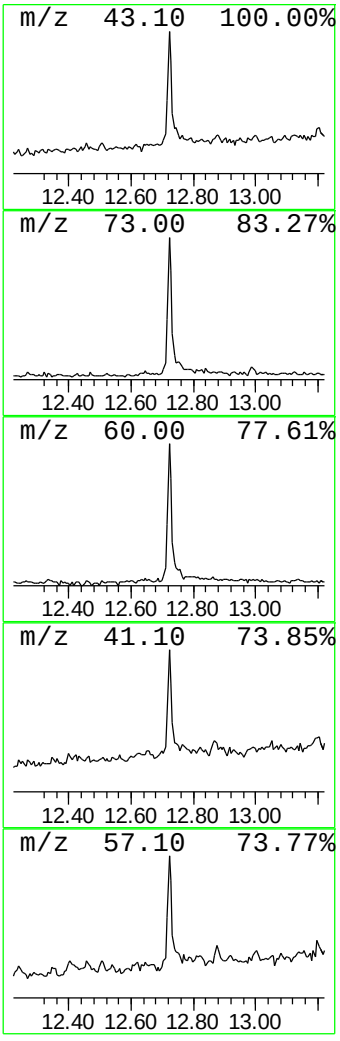
**********

Peak Number 5 Octadecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.72 | 3.28 ng | 242931 | Phenanthrene-d10 | 11.41 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 99 |
| 2 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 93 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 90 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 83 |
| 5 | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 74 |



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Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122018\
Data File : BF111645.D
Acq On : 20 Dec 2018 18:15
Operator : JU/SJ
Sample : J6353-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS003-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

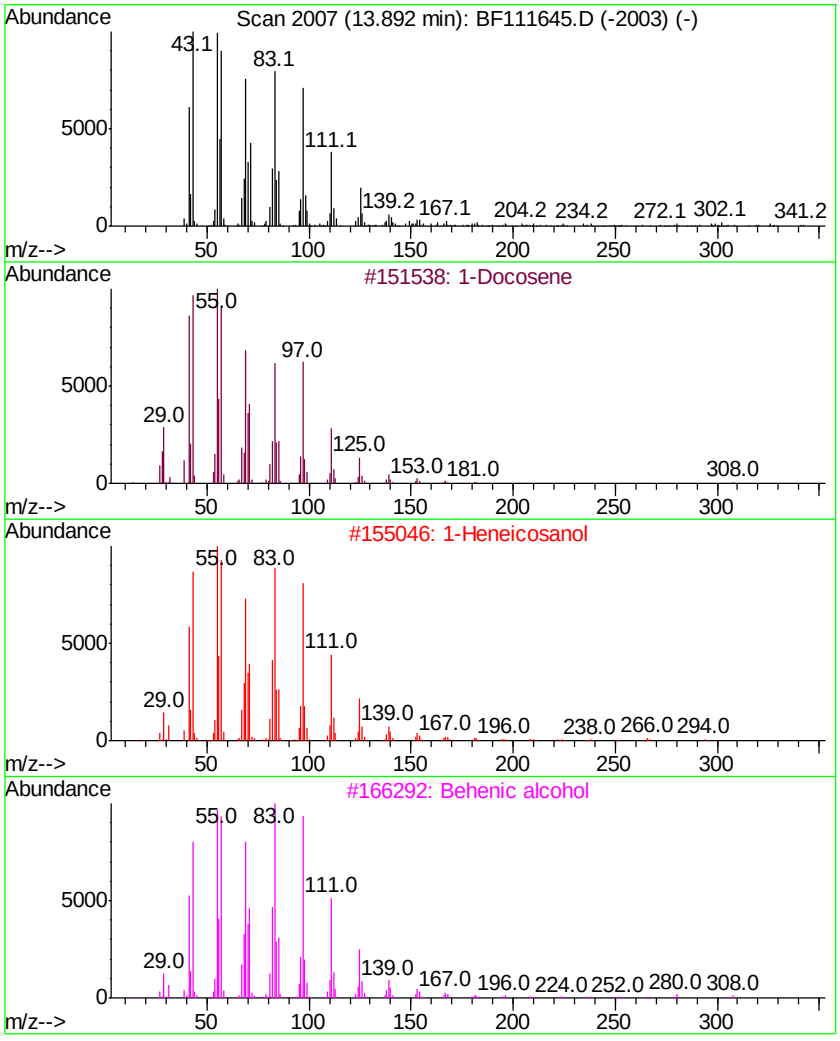
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

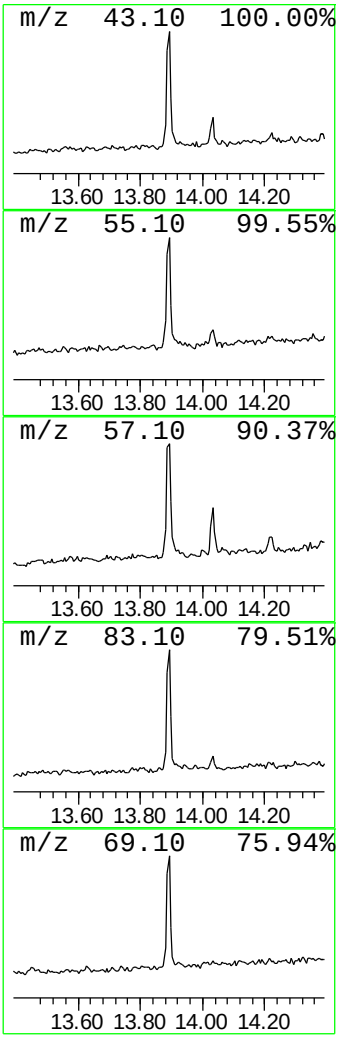
**********

Peak Number 6 1-Docosene Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.89 | 6.71 ng | 495403 | Chrysene-d12 | 14.04 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 96 |
| 2 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 95 |
| 3 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 95 |
| 4 | Cyclotetracosane | 336 | C24H48 | 000297-03-0 | 93 |
| 5 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 93 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF122018\
Data File : BF111645.D
Acq On : 20 Dec 2018 18:15
Operator : JU/SJ
Sample : J6353-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** P001-SS003-0002-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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... | 5.12 | 3.4 | ng | 207865 | 1 | 6.90 | 1230310 | 20.0 |
| unknown6.66 | 6.66 | 54.0 | ng | 3319880 | 1 | 6.90 | 1230310 | 20.0 |
| n-Hexadecanoic acid | 11.94 | 5.4 | ng | 403072 | 4 | 11.41 | 1482100 | 20.0 |
| Octadecanoic acid | 12.72 | 3.3 | ng | 242931 | 4 | 11.41 | 1482100 | 20.0 |
| 1-Docosene | 13.89 | 6.7 | ng | 495403 | 5 | 14.04 | 1475700 | 20.0 |