LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081018\
Data File : BF108095.D
Acq On : 10 Aug 2018 20:23
Operator : JU/SJ
Sample : J4272-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-03-080918-G

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-BF080818.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 | 5.248 | 491 | 495 | 503 | rVB | 616036 | 614435 | 4.76% | 0.877% |
| 2 | 5.637 | 556 | 561 | 564 | rBV | 3567347 | 3071735 | 23.81% | 4.383% |
| 3 | 6.631 | 725 | 730 | 733 | rBV | 3820217 | 3362532 | 26.07% | 4.798% |
| 4 | 6.784 | 752 | 756 | 760 | rBV | 3809311 | 3287985 | 25.49% | 4.691% |
| 5 | 7.019 | 792 | 796 | 799 | rBV | 2342991 | 1815758 | 14.08% | 2.591% |
| 6 | 7.172 | 819 | 822 | 826 | rVB | 2707469 | 2469071 | 19.14% | 3.523% |
| 7 | 7.578 | 886 | 891 | 894 | rBV | 2438542 | 2065486 | 16.01% | 2.947% |
| 8 | 8.301 | 1010 | 1014 | 1017 | rBV | 2758223 | 2231854 | 17.30% | 3.184% |
| 9 | 9.378 | 1192 | 1197 | 1200 | rBV | 4342600 | 3538128 | 27.43% | 5.048% |
| 10 | 9.766 | 1260 | 1263 | 1267 | rBV | 346705 | 282344 | 2.19% | 0.403% |
| 11 | 10.066 | 1310 | 1314 | 1318 | rBV | 2546647 | 2195504 | 17.02% | 3.133% |
| 12 | 10.478 | 1381 | 1384 | 1387 | rBV | 277116 | 214694 | 1.66% | 0.306% |
| 13 | 10.701 | 1417 | 1422 | 1424 | rBV | 158591 | 186724 | 1.45% | 0.266% |
| 14 | 10.860 | 1445 | 1449 | 1457 | rBV | 1732185 | 1745130 | 13.53% | 2.490% |
| 15 | 10.954 | 1462 | 1465 | 1471 | rBV | 432094 | 512952 | 3.98% | 0.732% |
| 16 | 11.407 | 1539 | 1542 | 1544 | rBV | 425407 | 350232 | 2.72% | 0.500% |
| 17 | 11.436 | 1544 | 1547 | 1549 | rVV | 176972 | 163697 | 1.27% | 0.234% |
| 18 | 11.566 | 1565 | 1569 | 1571 | rBV | 2174723 | 1882748 | 14.60% | 2.686% |
| 19 | 11.589 | 1571 | 1573 | 1577 | rVB | 188148 | 160550 | 1.24% | 0.229% |
| 20 | 11.830 | 1611 | 1614 | 1617 | rBV | 393517 | 326552 | 2.53% | 0.466% |
| 21 | 11.936 | 1628 | 1632 | 1635 | rVB | 4552635 | 3606724 | 27.96% | 5.146% |
| 22 | 12.066 | 1651 | 1654 | 1657 | rBV | 274304 | 276478 | 2.14% | 0.394% |
| 23 | 12.242 | 1681 | 1684 | 1686 | rBV | 369904 | 295502 | 2.29% | 0.422% |
| 24 | 12.636 | 1746 | 1751 | 1752 | rBV | 12567868 | 12899404 | 100.00% | 18.405% |
| 25 | 12.654 | 1752 | 1754 | 1760 | rVB2 | 11543266 | 11126856 | 86.26% | 15.876% |
| 26 | 12.730 | 1764 | 1767 | 1771 | rBV | 2464654 | 2275615 | 17.64% | 3.247% |
| 27 | 12.783 | 1771 | 1776 | 1779 | rBV | 538768 | 548385 | 4.25% | 0.782% |
| 28 | 12.972 | 1805 | 1808 | 1811 | rBV | 342512 | 298672 | 2.32% | 0.426% |
| 29 | 13.013 | 1811 | 1815 | 1821 | rVB2 | 395411 | 586468 | 4.55% | 0.837% |
| 30 | 13.154 | 1835 | 1839 | 1842 | rBV | 3239731 | 2724976 | 21.12% | 3.888% |
| 31 | 13.301 | 1861 | 1864 | 1866 | rBV | 355625 | 377981 | 2.93% | 0.539% |
| 32 | 13.366 | 1873 | 1875 | 1877 | rBV | 207914 | 172479 | 1.34% | 0.246% |
| 33 | 13.460 | 1888 | 1891 | 1894 | rBV2 | 341955 | 297687 | 2.31% | 0.425% |
| 34 | 13.571 | 1907 | 1910 | 1914 | rBV2 | 362654 | 369425 | 2.86% | 0.527% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081018\
Data File : BF108095.D
Acq On : 10 Aug 2018 20:23
Operator : JU/SJ
Sample : J4272-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-03-080918-G

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-BF080818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 13.889 | 1961 | 1964 | 1968 | rVB2 | 244337 | 322636 | 2.50% | 0.460% |
| 36 | 14.130 | 2003 | 2005 | 2009 | rBV | 258285 | 260187 | 2.02% | 0.371% |
| 37 | 14.218 | 2016 | 2020 | 2023 | rBV | 1804477 | 1918609 | 14.87% | 2.738% |
| 38 | 15.789 | 2283 | 2287 | 2293 | rVB | 915337 | 1249621 | 9.69% | 1.783% |

Sum of corrected areas: 70085816

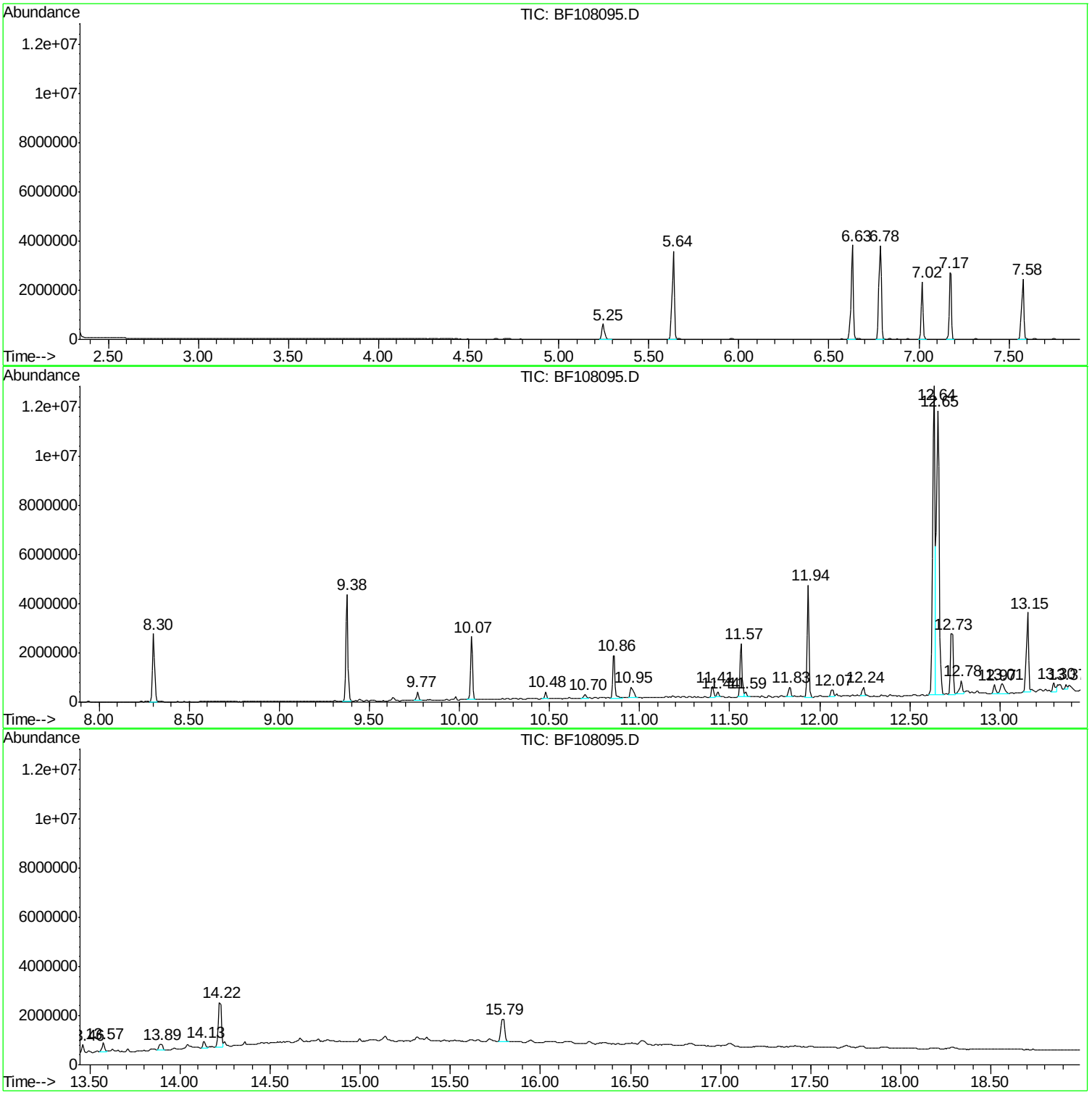
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081018\
Data File : BF108095.D
Acq On : 10 Aug 2018 20:23
Operator : JU/SJ
Sample : J4272-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-03-080918-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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\BF081018\
Data File : BF108095.D
Acq On : 10 Aug 2018 20:23
Operator : JU/SJ
Sample : J4272-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-03-080918-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

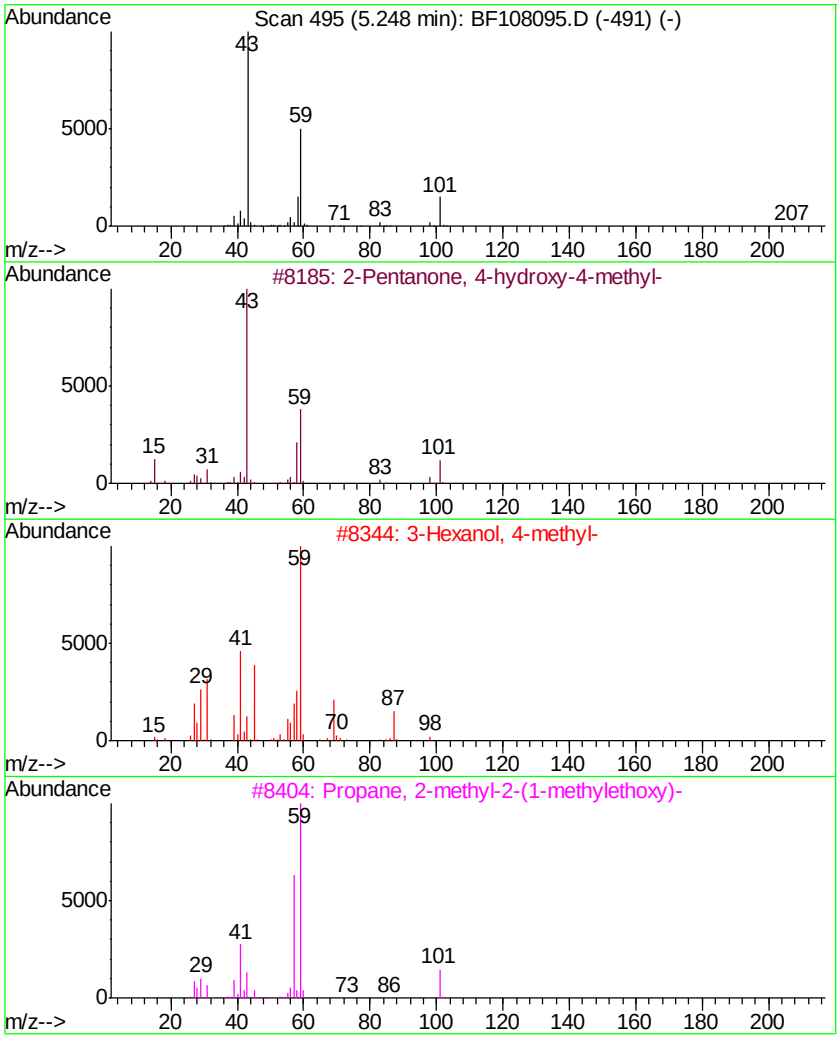
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

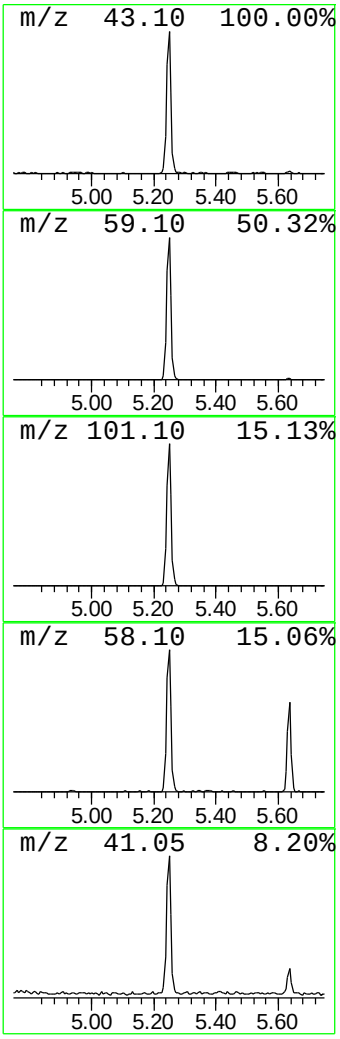
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.25 | 6.77 ng | 614435 | 1,4-Dichlorobenzene-d4 | 7.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 3 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 33 |
| 4 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |
| 5 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 10 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081018\
Data File : BF108095.D
Acq On : 10 Aug 2018 20:23
Operator : JU/SJ
Sample : J4272-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-03-080918-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

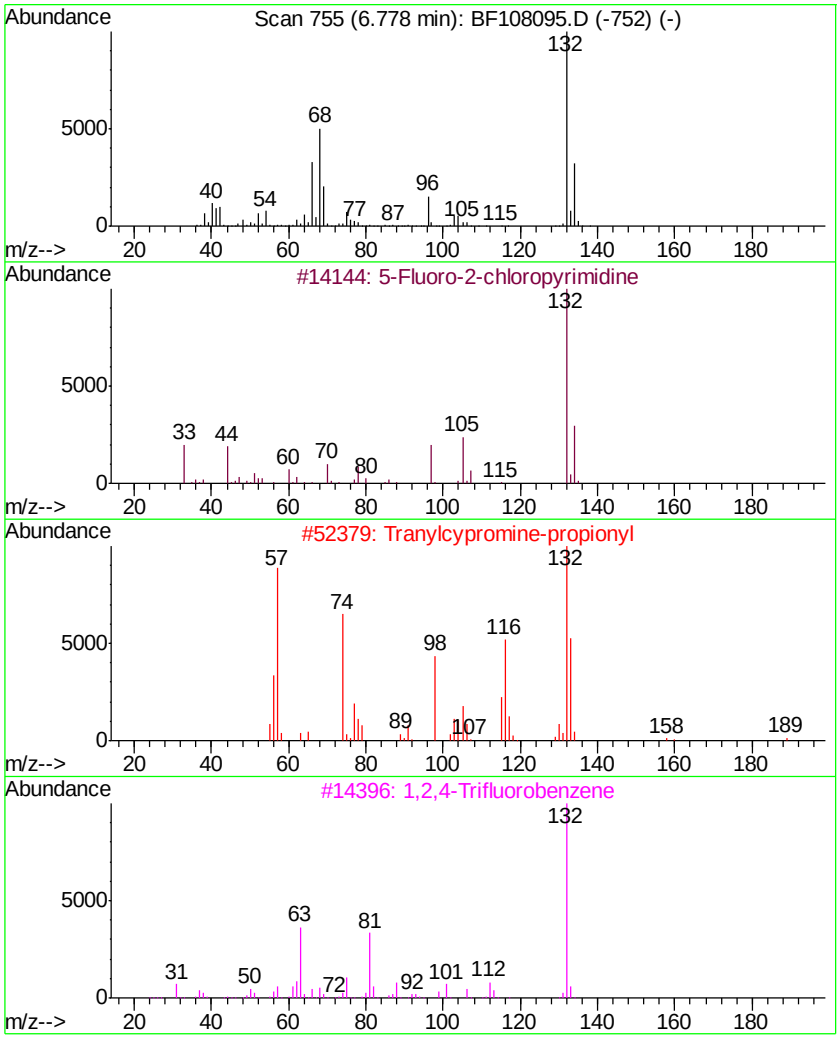
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

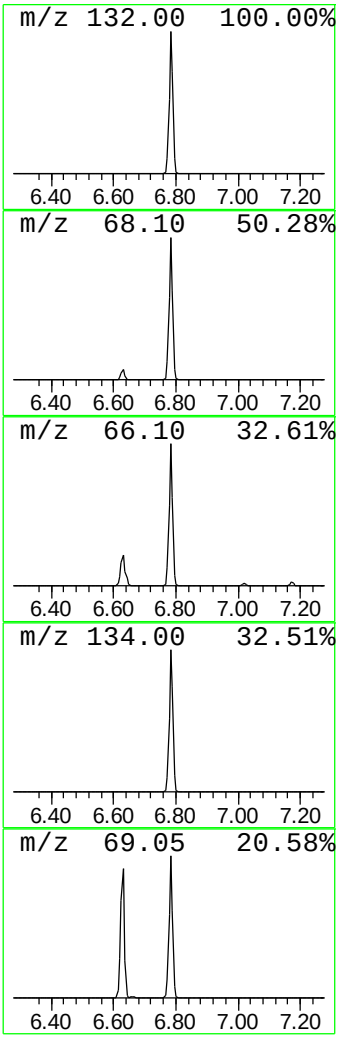
**********

Peak Number 2 unknown6.78 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.78 | 36.22 ng | 3287990 | 1,4-Dichlorobenzene-d4 | 7.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 2 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 3 | 1,2,4-Trifluorobenzene | 132 | C6H3F3 | 000367-23-7 | 9 |
| 4 | 1,3,5-Trifluorobenzene | 132 | C6H3F3 | 000372-38-3 | 9 |
| 5 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081018\
Data File : BF108095.D
Acq On : 10 Aug 2018 20:23
Operator : JU/SJ
Sample : J4272-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-03-080918-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

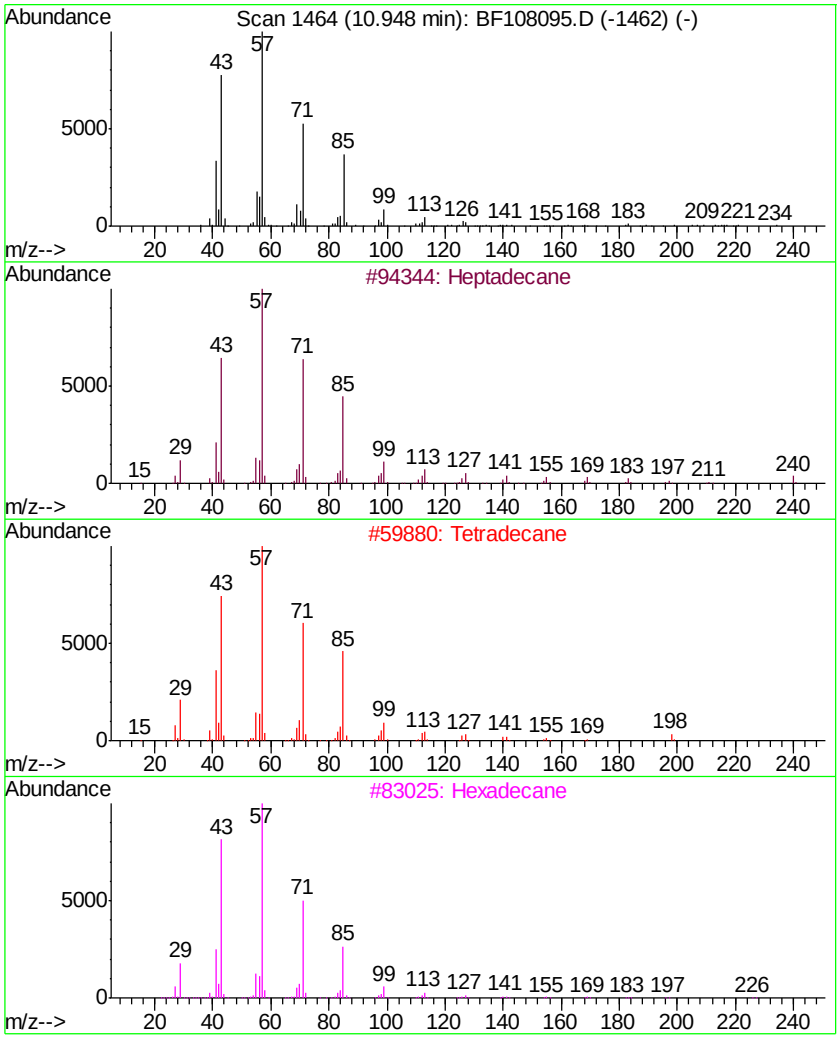
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

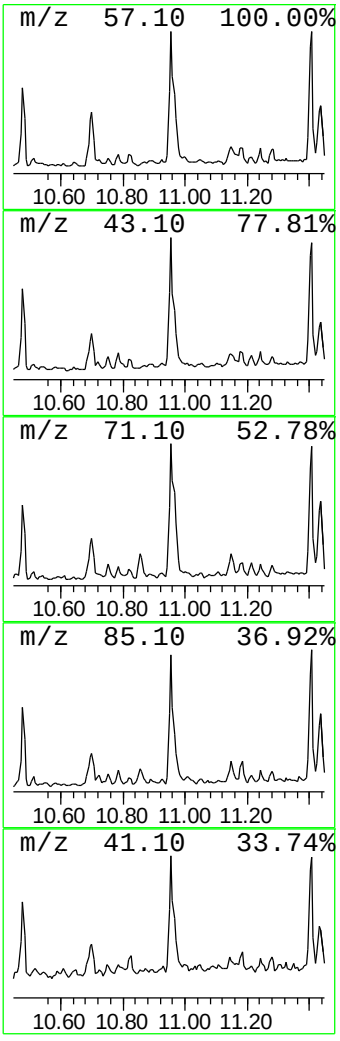
**********

Peak Number 4 Heptadecane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.95 | 5.45 ng | 512952 | Phenanthrene-d10 | 11.57 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane | 240 | C17H36 | 000629-78-7 | 91 |
| 2 | Tetradecane | 198 | C14H30 | 000629-59-4 | 90 |
| 3 | Hexadecane | 226 | C16H34 | 000544-76-3 | 90 |
| 4 | Pentadecane | 212 | C15H32 | 000629-62-9 | 90 |
| 5 | Dodecane, 2-methyl-6-propyl- | 226 | C16H34 | 055045-08-4 | 86 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081018\
Data File : BF108095.D
Acq On : 10 Aug 2018 20:23
Operator : JU/SJ
Sample : J4272-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-03-080918-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

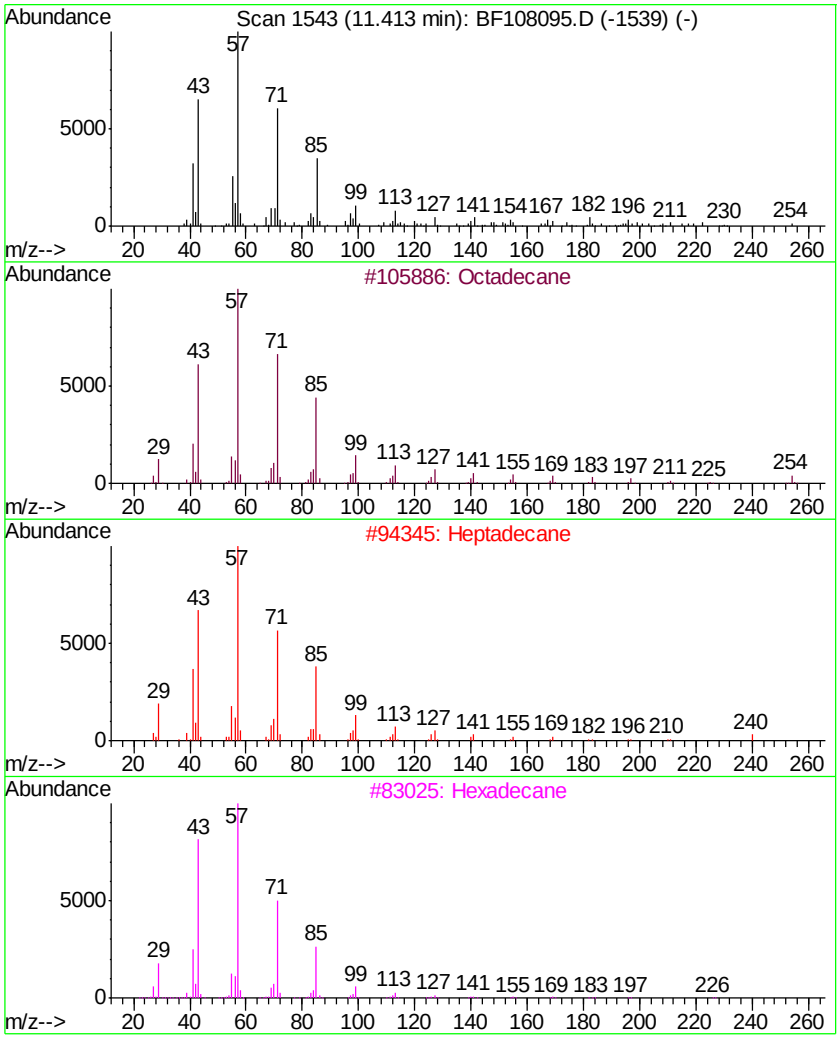
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

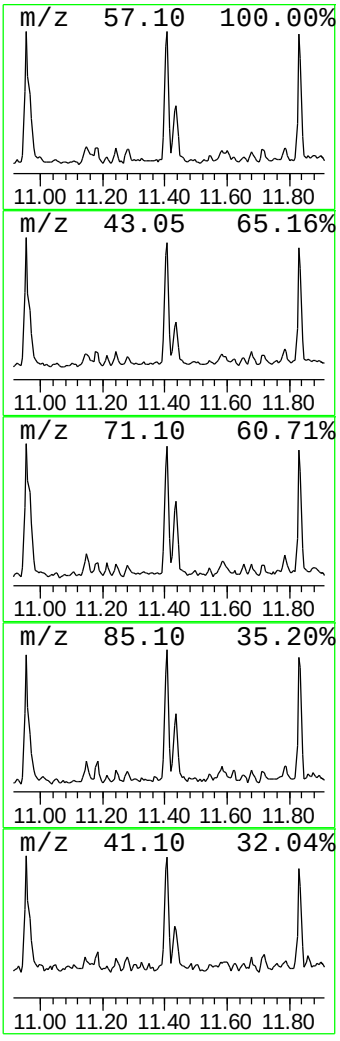
**********

Peak Number 5 Octadecane Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.41 | 3.72 ng | 350232 | Phenanthrene-d10 | 11.57 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecane | 254 | C18H38 | 000593-45-3 | 97 |
| 2 | Heptadecane | 240 | C17H36 | 000629-78-7 | 90 |
| 3 | Hexadecane | 226 | C16H34 | 000544-76-3 | 90 |
| 4 | Tetracosane | 338 | C24H50 | 000646-31-1 | 90 |
| 5 | Pentadecane | 212 | C15H32 | 000629-62-9 | 90 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081018\
Data File : BF108095.D
Acq On : 10 Aug 2018 20:23
Operator : JU/SJ
Sample : J4272-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-03-080918-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

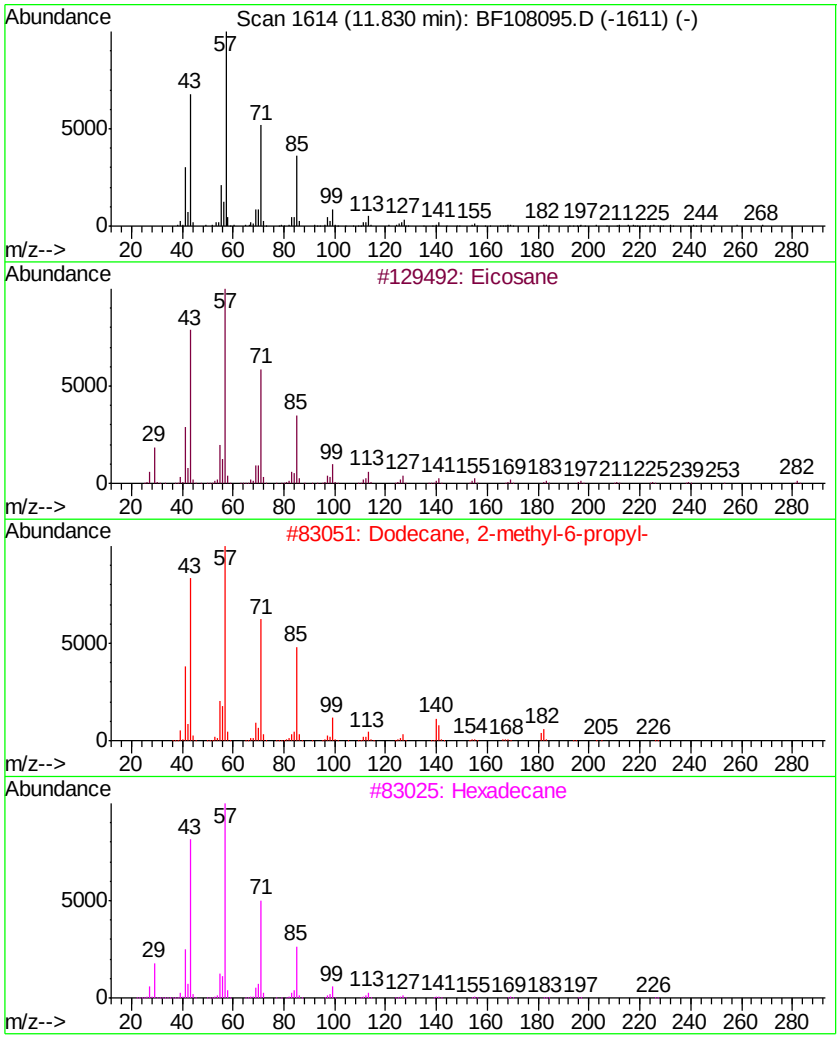
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

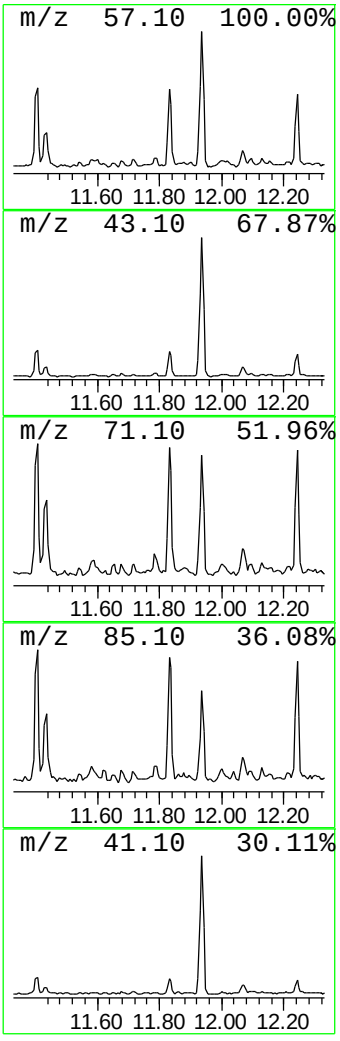
**********

Peak Number 6 Eicosane Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.83 | 3.47 ng | 326552 | Phenanthrene-d10 | 11.57 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 90 |
| 2 | Dodecane, 2-methyl-6-propyl- | 226 | C16H34 | 055045-08-4 | 86 |
| 3 | Hexadecane | 226 | C16H34 | 000544-76-3 | 86 |
| 4 | Heptacosane | 380 | C27H56 | 000593-49-7 | 83 |
| 5 | Tridecane | 184 | C13H28 | 000629-50-5 | 81 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081018\
Data File : BF108095.D
Acq On : 10 Aug 2018 20:23
Operator : JU/SJ
Sample : J4272-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-03-080918-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

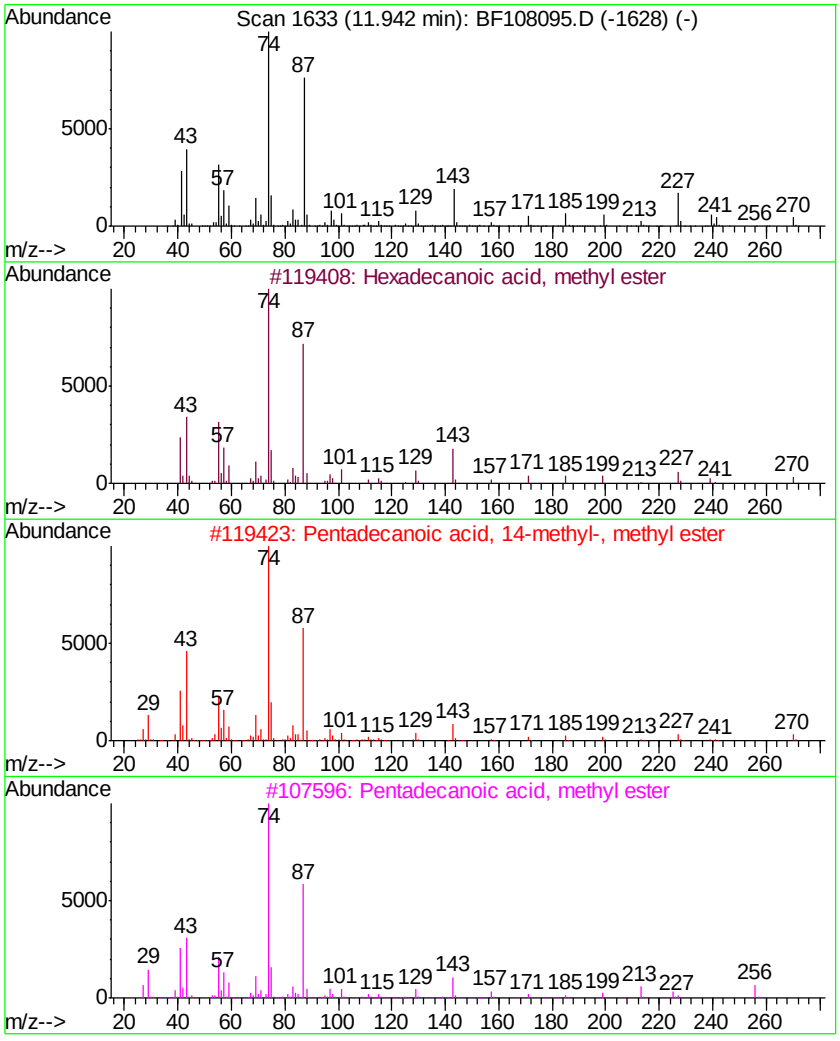
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

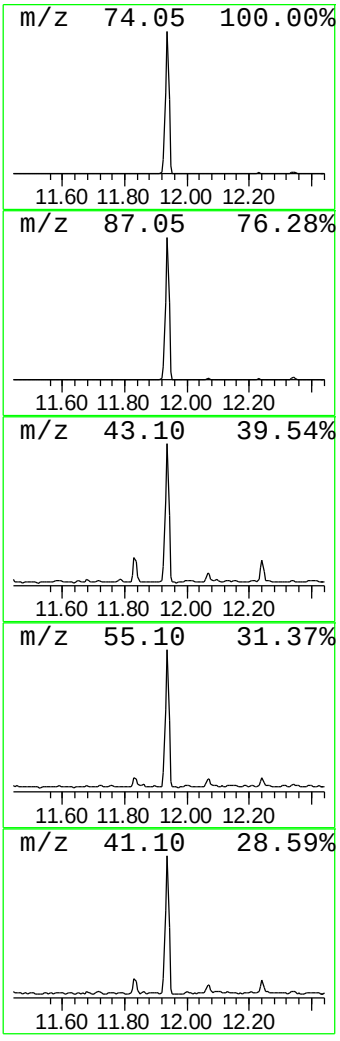
**********

Peak Number 7 Hexadecanoic acid, methyl e... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.94 | 38.31 ng | 3606720 | Phenanthrene-d10 | 11.57 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecanoic acid, methyl ester | 270 | C17H34O2 | 000112-39-0 | 98 |
| 2 | Pentadecanoic acid, 14-methyl-, ... | 270 | C17H34O2 | 005129-60-2 | 96 |
| 3 | Pentadecanoic acid, methyl ester | 256 | C16H32O2 | 007132-64-1 | 86 |
| 4 | Hexadecanoic acid, 15-methyl-, m... | 284 | C18H36O2 | 006929-04-0 | 83 |
| 5 | Tridecanoic acid, 12-methyl-, me... | 242 | C15H30O2 | 005129-58-8 | 80 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081018\
Data File : BF108095.D
Acq On : 10 Aug 2018 20:23
Operator : JU/SJ
Sample : J4272-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-03-080918-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

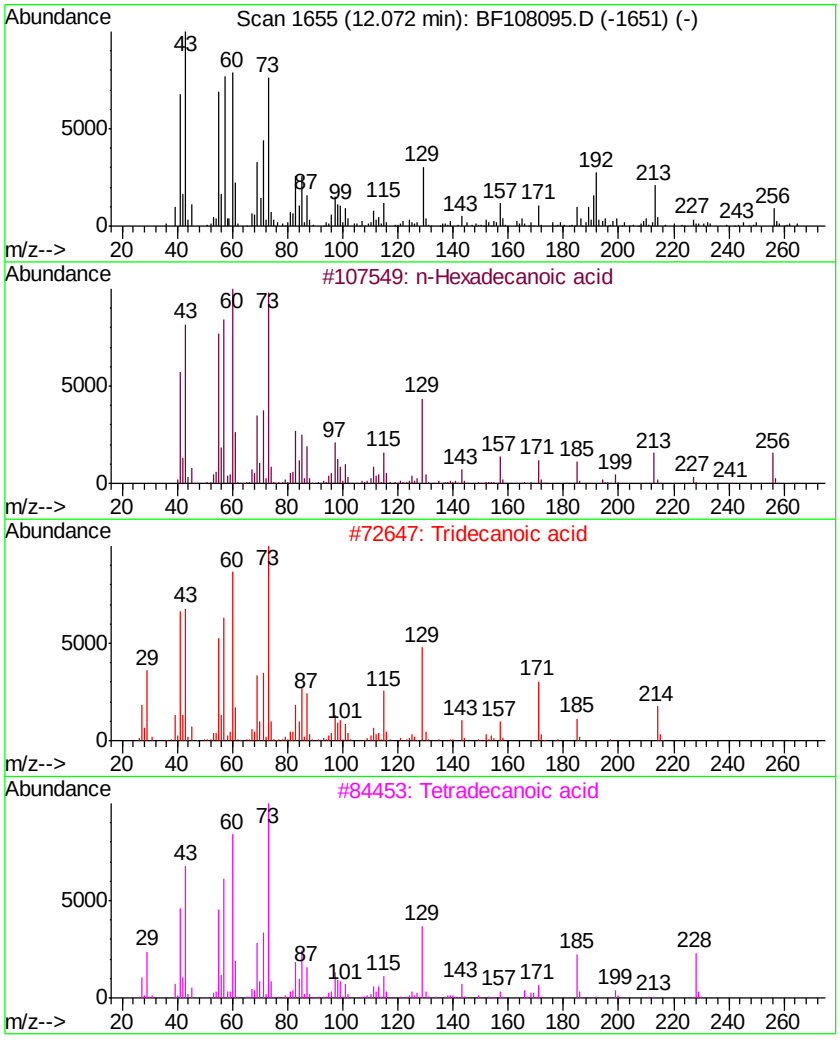
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

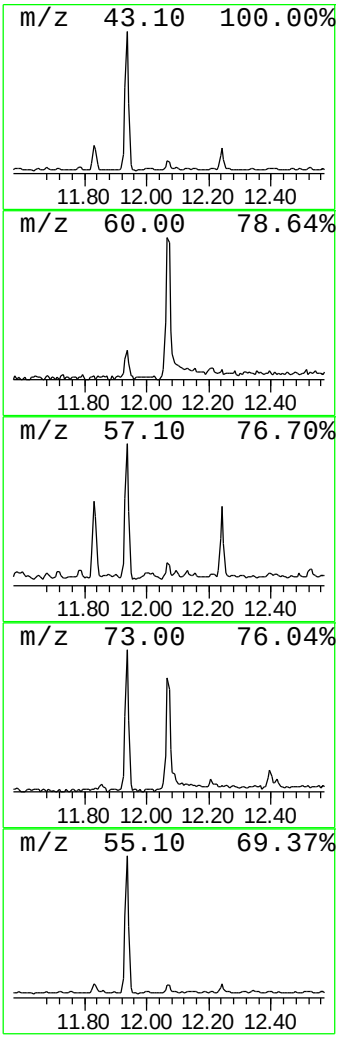
**********

Peak Number 8 n-Hexadecanoic acid Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.07 | 2.94 ng | 276478 | Phenanthrene-d10 | 11.57 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 95 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 50 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 46 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 43 |
| 5 | Isoamyl nitrite | 117 | C5H11NO2 | 000110-46-3 | 22 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081018\
Data File : BF108095.D
Acq On : 10 Aug 2018 20:23
Operator : JU/SJ
Sample : J4272-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-03-080918-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

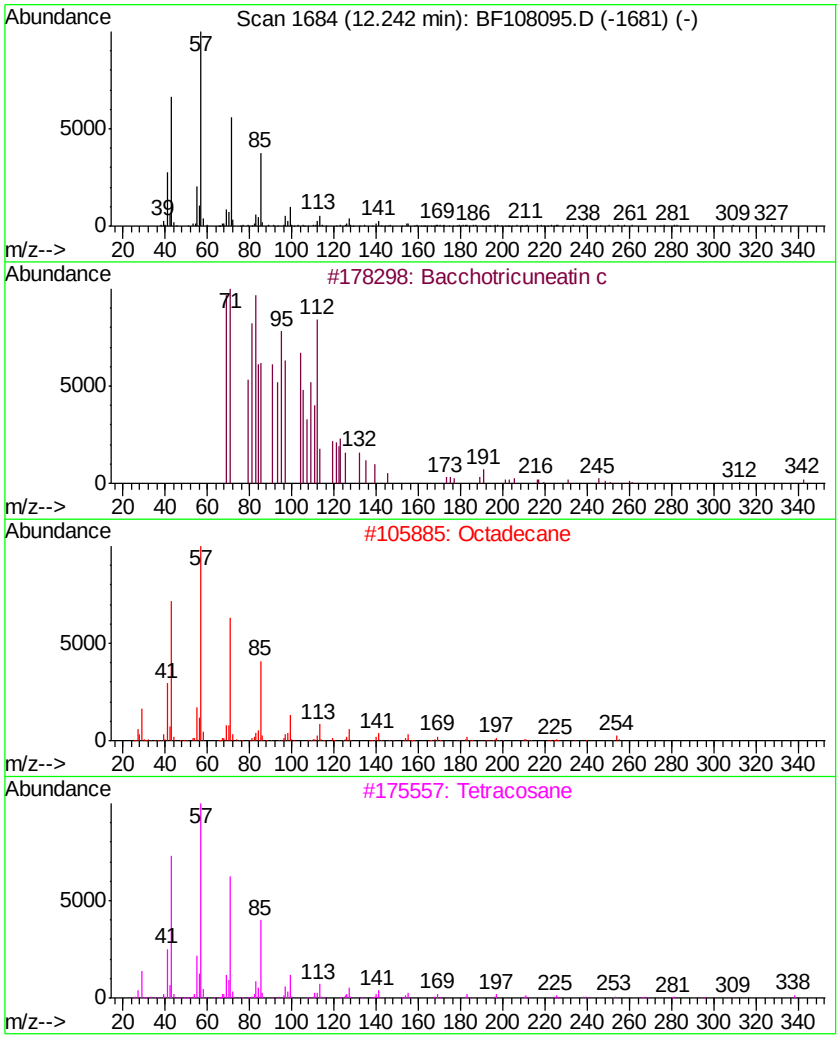
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

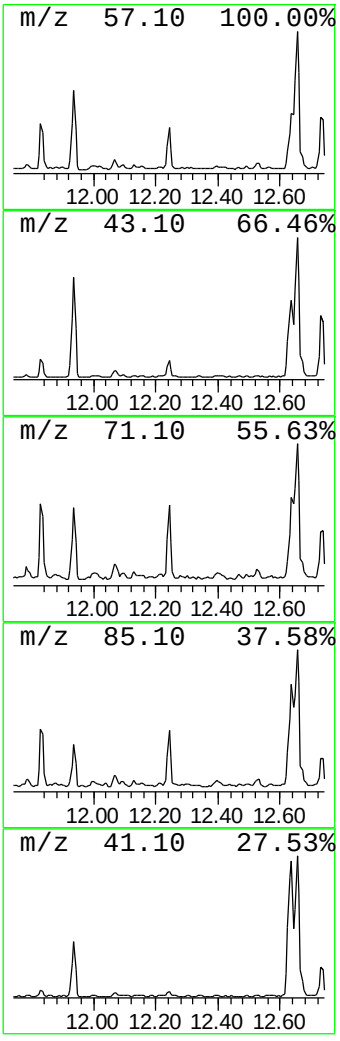
**********

Peak Number 9 Bacchotricuneatin c Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.24 | 3.14 ng | 295502 | Phenanthrene-d10 | 11.57 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Bacchotricuneatin c | 342 | C20H22O5 | 066563-30-2 | 98 |
| 2 | Octadecane | 254 | C18H38 | 000593-45-3 | 94 |
| 3 | Tetracosane | 338 | C24H50 | 000646-31-1 | 91 |
| 4 | Eicosane | 282 | C20H42 | 000112-95-8 | 90 |
| 5 | Pentadecane, 7-methyl- | 226 | C16H34 | 006165-40-8 | 90 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081018\
Data File : BF108095.D
Acq On : 10 Aug 2018 20:23
Operator : JU/SJ
Sample : J4272-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-03-080918-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

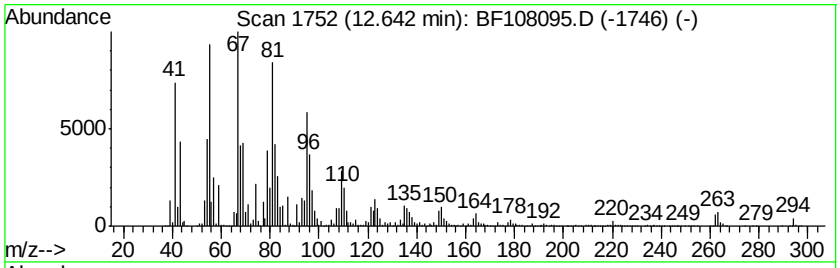
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

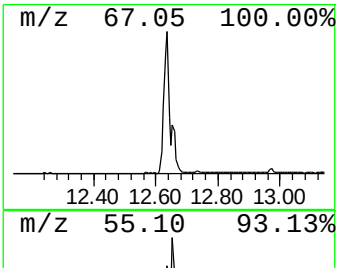
**********

Peak Number 10 9,12-Octadecadienoic acid, ... Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.64 | 137.03 ng | 12899400 | Phenanthrene-d10 | 11.57 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9,12-Octadecadienoic acid, methy... | 294 | C19H34O2 | 002566-97-4 | 99 |
| 2 | 9,12-Octadecadienoic acid, methy... | 294 | C19H34O2 | 002462-85-3 | 99 |
| 3 | 9,15-Octadecadienoic acid, methy... | 294 | C19H34O2 | 017309-05-6 | 99 |
| 4 | Methyl 9-cis,11-trans-octadecadi... | 294 | C19H34O2 | 1000336-44-0 | 99 |
| 5 | 9,12-Octadecadienoic acid (Z,Z)-... | 294 | C19H34O2 | 000112-63-0 | 98 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081018\
Data File : BF108095.D
Acq On : 10 Aug 2018 20:23
Operator : JU/SJ
Sample : J4272-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-03-080918-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

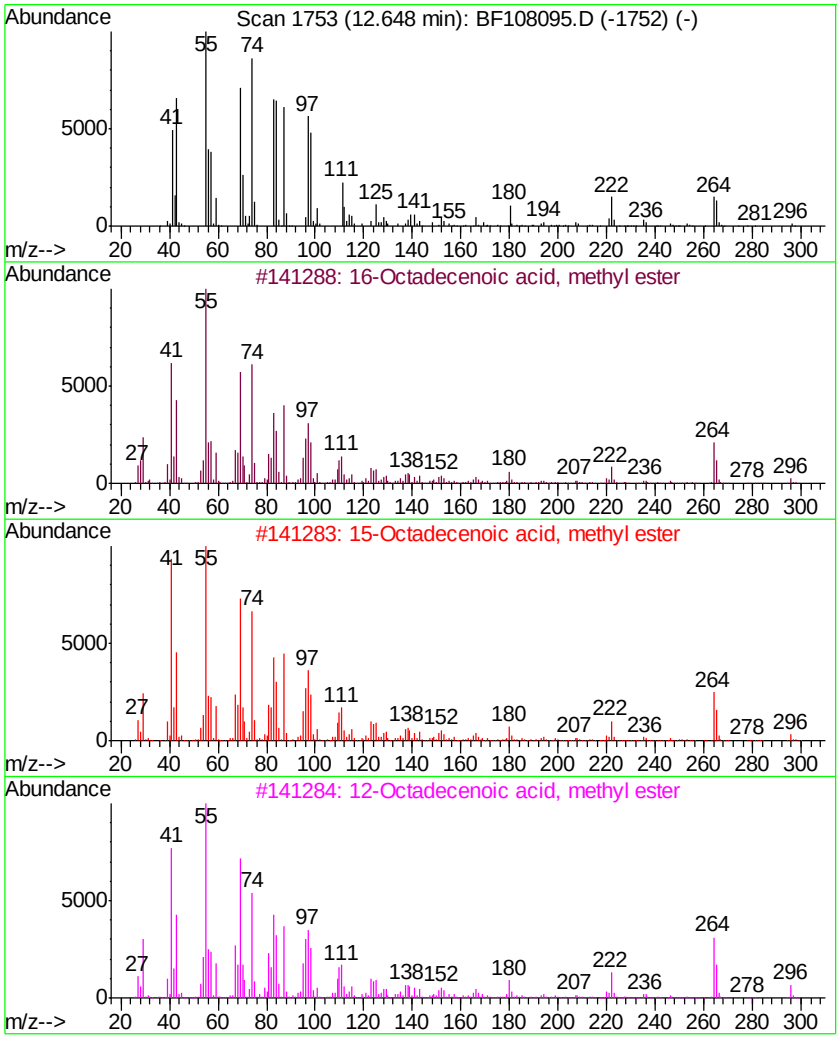
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

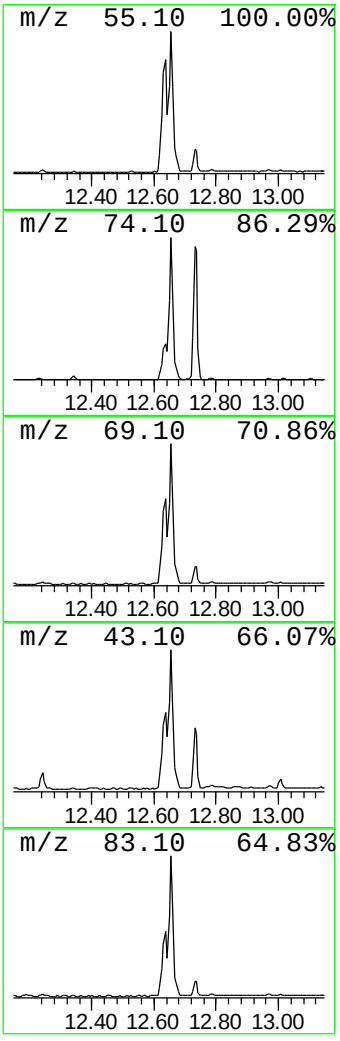
**********

Peak Number 11 16-Octadecenoic acid, methy... Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.65 | 118.20 ng | 11126900 | Phenanthrene-d10 | 11.57 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 16-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 056554-49-5 | 95 |
| 2 | 15-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 004764-72-1 | 93 |
| 3 | 12-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 056554-46-2 | 93 |
| 4 | 13-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 056554-47-3 | 90 |
| 5 | 14-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 056554-48-4 | 87 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081018\
Data File : BF108095.D
Acq On : 10 Aug 2018 20:23
Operator : JU/SJ
Sample : J4272-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-03-080918-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

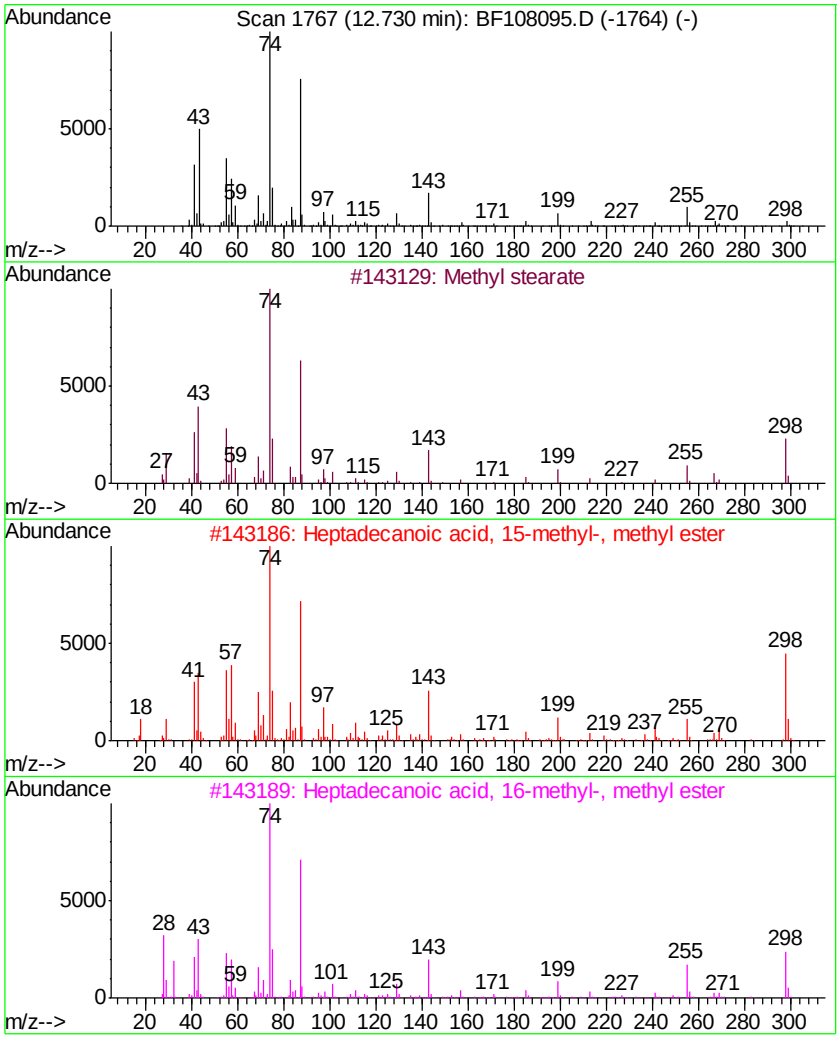
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

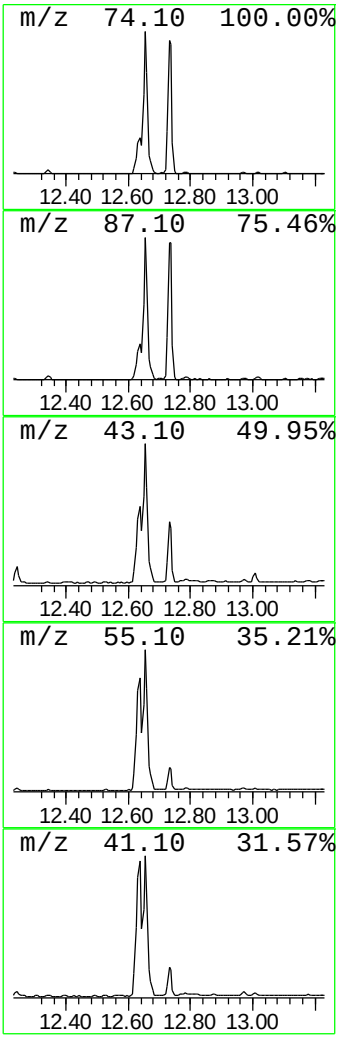
**********

Peak Number 12 Methyl stearate Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.73 | 24.17 ng | 2275620 | Phenanthrene-d10 | 11.57 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methyl stearate | 298 | C19H38O2 | 000112-61-8 | 97 |
| 2 | Heptadecanoic acid, 15-methyl-, ... | 298 | C19H38O2 | 054833-55-5 | 93 |
| 3 | Heptadecanoic acid, 16-methyl-, ... | 298 | C19H38O2 | 005129-61-3 | 92 |
| 4 | Heptadecanoic acid, methyl ester | 284 | C18H36O2 | 001731-92-6 | 91 |
| 5 | Hexadecanoic acid, methyl ester | 270 | C17H34O2 | 000112-39-0 | 90 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081018\
Data File : BF108095.D
Acq On : 10 Aug 2018 20:23
Operator : JU/SJ
Sample : J4272-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-03-080918-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

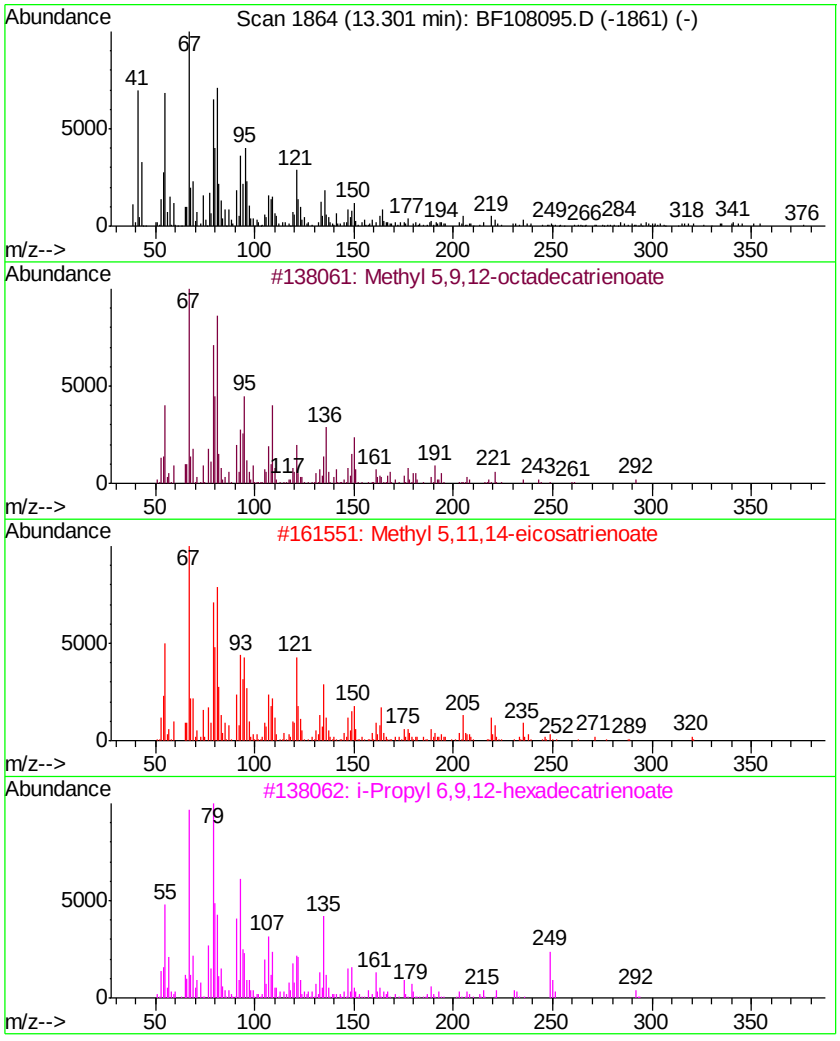
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

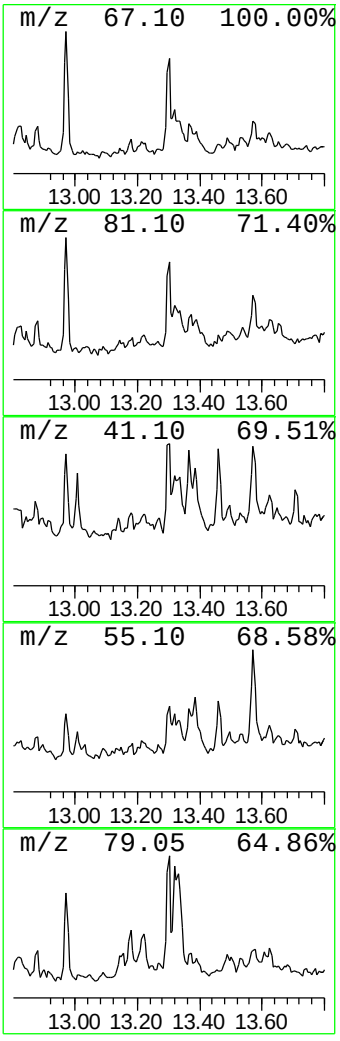
**********

Peak Number 13 Methyl 5,9,12-octadecatrien... Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.30 | 3.94 ng | 377981 | Chrysene-d12 | 14.22 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methyl 5,9,12-octadecatrienoate | 292 | C19H32O2 | 1000336-37-5 | 91 |
| 2 | Methyl 5,11,14-eicosatrienoate | 320 | C21H36O2 | 1000336-40-2 | 90 |
| 3 | i-Propyl 6,9,12-hexadecatrienoate | 292 | C19H32O2 | 1000336-78-1 | 86 |
| 4 | Methyl 9,10-octadecadienoate | 294 | C19H34O2 | 1000336-45-7 | 64 |
| 5 | 1,6-Cyclodecadiene | 136 | C10H16 | 007049-13-0 | 64 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081018\
Data File : BF108095.D
Acq On : 10 Aug 2018 20:23
Operator : JU/SJ
Sample : J4272-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-03-080918-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

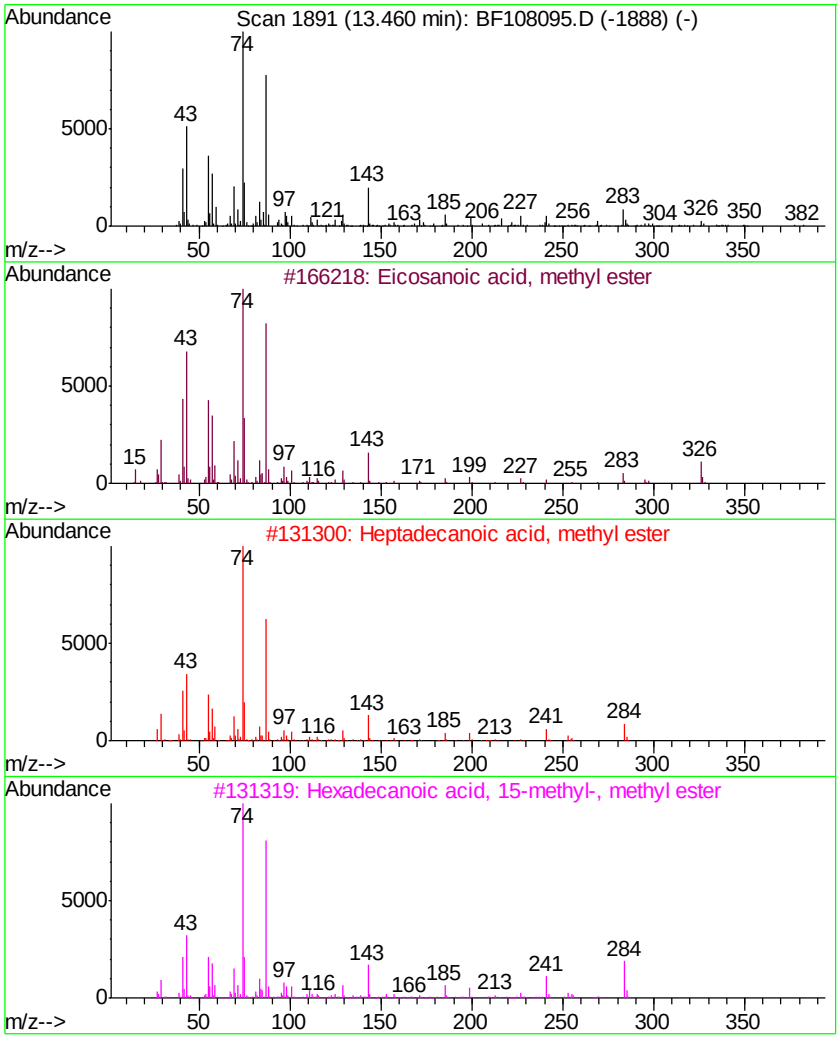
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

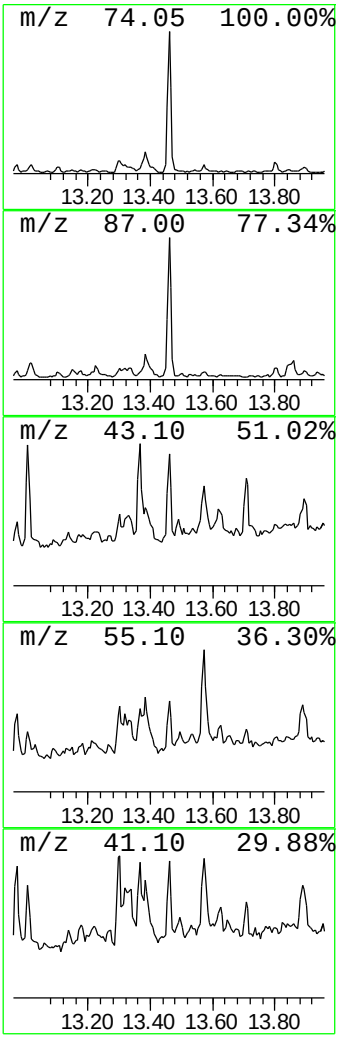
**********

Peak Number 14 Eicosanoic acid, methyl ester Concentration Rank 15

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.46 | 3.10 ng | 297687 | Chrysene-d12 | 14.22 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosanoic acid, methyl ester | 326 | C21H42O2 | 001120-28-1 | 95 |
| 2 | Heptadecanoic acid, methyl ester | 284 | C18H36O2 | 001731-92-6 | 93 |
| 3 | Hexadecanoic acid, 15-methyl-, m... | 284 | C18H36O2 | 006929-04-0 | 93 |
| 4 | Hexadecanoic acid, 14-methyl-, m... | 284 | C18H36O2 | 002490-49-5 | 90 |
| 5 | Methyl stearate | 298 | C19H38O2 | 000112-61-8 | 87 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081018\
Data File : BF108095.D
Acq On : 10 Aug 2018 20:23
Operator : JU/SJ
Sample : J4272-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-03-080918-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

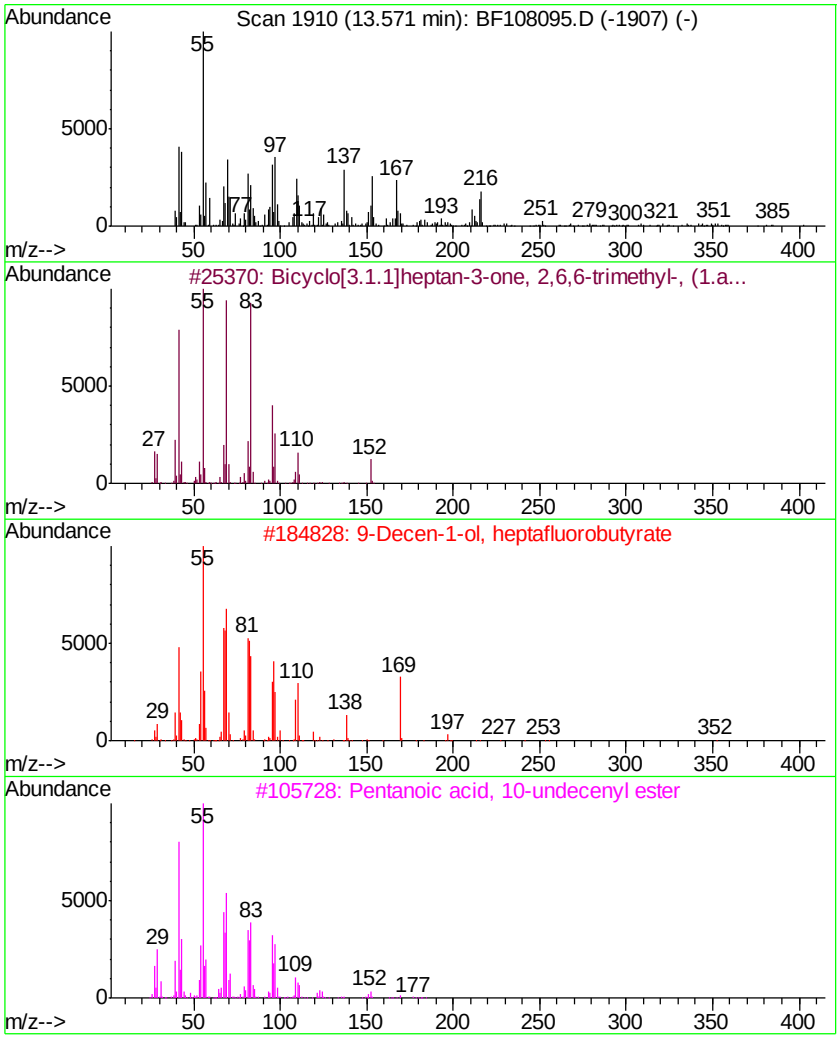
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

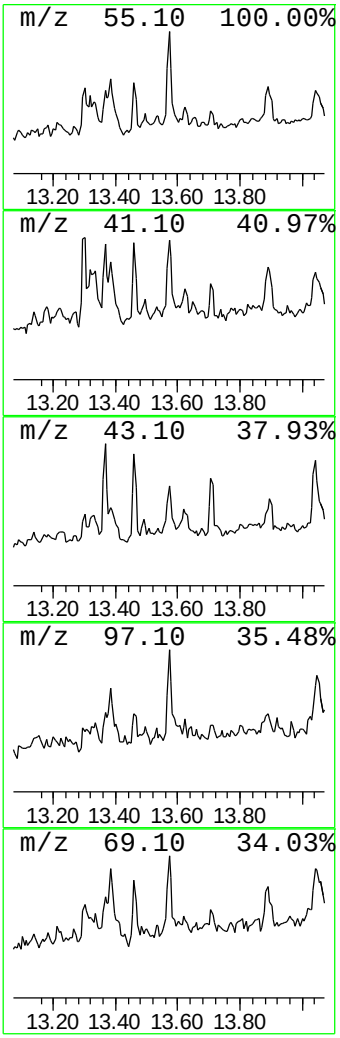
**********

Peak Number 15 unknown13.57 Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.57 | 3.85 ng | 369425 | Chrysene-d12 | 14.22 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Bicyclo[3.1.1]heptan-3-one, 2,6,... | 152 | C10H16O | 000547-60-4 | 35 |
| 2 | 9-Decen-1-ol, heptafluorobutyrate | 352 | C14H19F7O2 | 1000352-65-4 | 16 |
| 3 | Pentanoic acid, 10-undecenyl ester | 254 | C16H30O2 | 1000159-93-4 | 14 |
| 4 | (R)-(-)-(Z)-14-Methyl-8-hexadece... | 254 | C17H34O | 030689-78-2 | 12 |
| 5 | Thiomescaline | 227 | C11H17NO2S | 1000379-13-6 | 10 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081018\
Data File : BF108095.D
Acq On : 10 Aug 2018 20:23
Operator : JU/SJ
Sample : J4272-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-03-080918-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

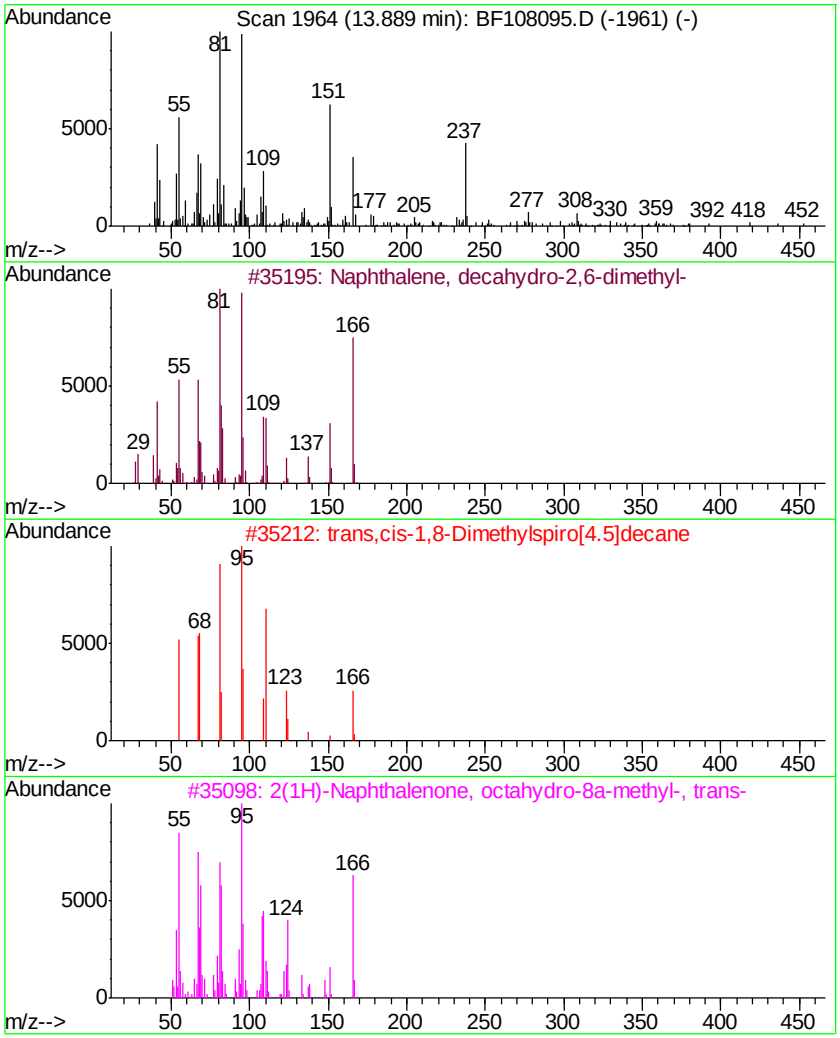
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

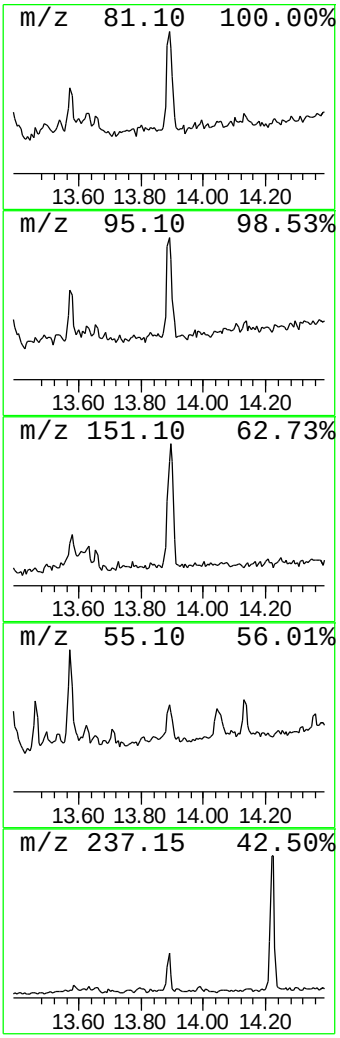
**********

Peak Number 16 Naphthalene, decahydro-2,6-... Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.89 | 3.36 ng | 322636 | Chrysene-d12 | 14.22 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Naphthalene, decahydro-2,6-dimet... | 166 | C12H22 | 001618-22-0 | 68 |
| 2 | trans,cis-1,8-Dimethylspiro[4.5]... | 166 | C12H22 | 1000111-72-9 | 52 |
| 3 | 2(1H)-Naphthalenone, octahydro-8... | 166 | C11H18O | 001197-95-1 | 22 |
| 4 | 5,7-Octadien-4-one, 2,6-dimethyl... | 152 | C10H16O | 003588-18-9 | 18 |
| 5 | 4-Isopropylbenzenethiol, S-methyl- | 166 | C10H14S | 1000353-04-8 | 15 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081018\
Data File : BF108095.D
Acq On : 10 Aug 2018 20:23
Operator : JU/SJ
Sample : J4272-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-03-080918-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

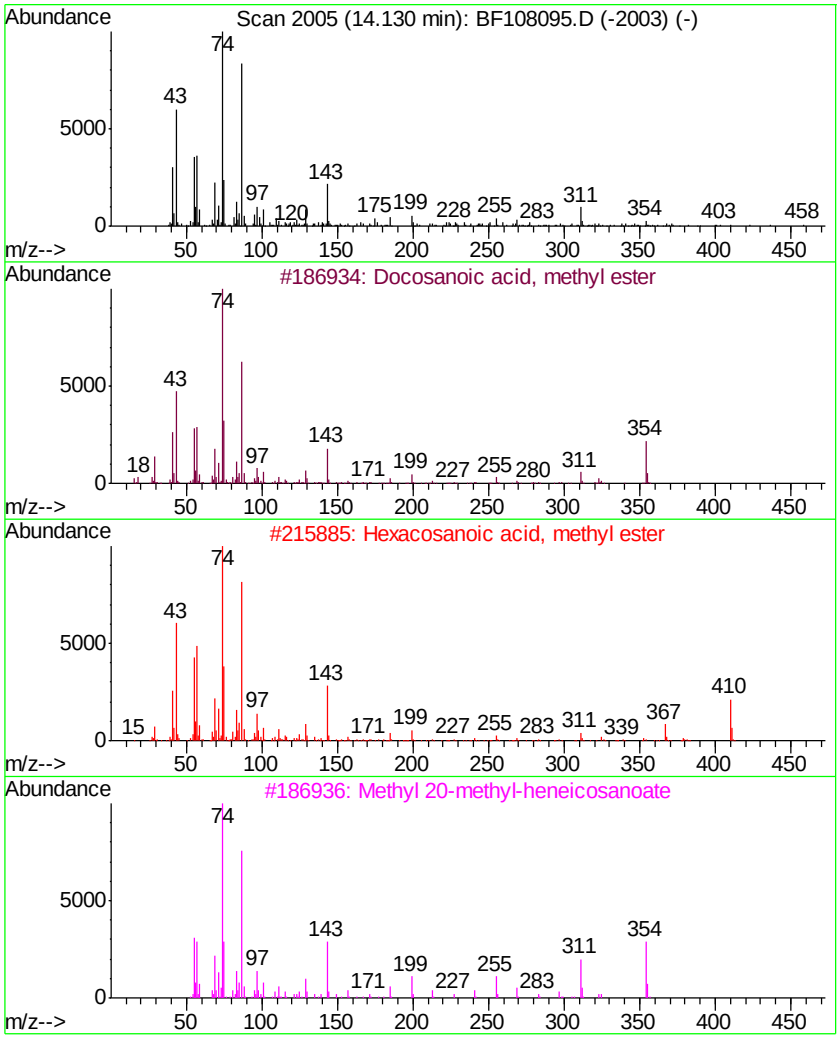
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

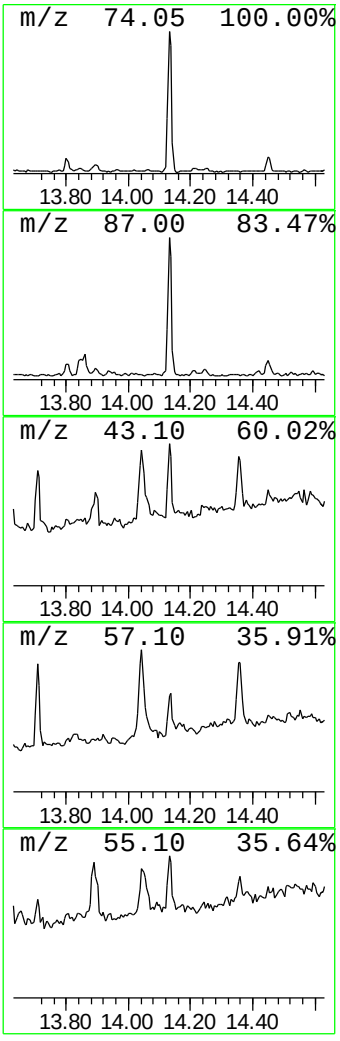
**********

Peak Number 17 Docosanoic acid, methyl ester Concentration Rank 17

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.13 | 2.71 ng | 260187 | Chrysene-d12 | 14.22 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Docosanoic acid, methyl ester | 354 | C23H46O2 | 000929-77-1 | 95 |
| 2 | Hexacosanoic acid, methyl ester | 410 | C27H54O2 | 005802-82-4 | 91 |
| 3 | Methyl 20-methyl-heneicosanoate | 354 | C23H46O2 | 1000336-47-4 | 89 |
| 4 | Hexadecanoic acid, methyl ester | 270 | C17H34O2 | 000112-39-0 | 87 |
| 5 | Methyl 9-methyltetradecanoate | 256 | C16H32O2 | 213617-69-7 | 86 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081018\
Data File : BF108095.D
Acq On : 10 Aug 2018 20:23
Operator : JU/SJ
Sample : J4272-13 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** JC-03-080918-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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... | 5.25 | 6.8 | ng | 614435 | 1 | 7.02 | 1815760 | 20.0 |
| unknown6.78 | 6.78 | 36.2 | ng | 3287990 | 1 | 7.02 | 1815760 | 20.0 |
| Heptadecane | 10.95 | 5.5 | ng | 512952 | 4 | 11.57 | 1882750 | 20.0 |
| Octadecane | 11.41 | 3.7 | ng | 350232 | 4 | 11.57 | 1882750 | 20.0 |
| Eicosane | 11.83 | 3.5 | ng | 326552 | 4 | 11.57 | 1882750 | 20.0 |
| Hexadecanoic acid... | 11.94 | 38.3 | ng | 3606720 | 4 | 11.57 | 1882750 | 20.0 |
| n-Hexadecanoic acid | 12.07 | 2.9 | ng | 276478 | 4 | 11.57 | 1882750 | 20.0 |
| Bacchotricuneatin c | 12.24 | 3.1 | ng | 295502 | 4 | 11.57 | 1882750 | 20.0 |
| 9,12-Octadecadien... | 12.64 | 137.0 | ng | 12899400 | 4 | 11.57 | 1882750 | 20.0 |
| 16-Octadecenoic a... | 12.65 | 118.2 | ng | 11126900 | 4 | 11.57 | 1882750 | 20.0 |
| Methyl stearate | 12.73 | 24.2 | ng | 2275620 | 4 | 11.57 | 1882750 | 20.0 |
| Methyl 5,9,12-oct... | 13.30 | 3.9 | ng | 377981 | 5 | 14.22 | 1918610 | 20.0 |
| Eicosanoic acid, ... | 13.46 | 3.1 | ng | 297687 | 5 | 14.22 | 1918610 | 20.0 |
| unknown13.57 | 13.57 | 3.9 | ng | 369425 | 5 | 14.22 | 1918610 | 20.0 |
| Naphthalene, deca... | 13.89 | 3.4 | ng | 322636 | 5 | 14.22 | 1918610 | 20.0 |
| Docosanoic acid, ... | 14.13 | 2.7 | ng | 260187 | 5 | 14.22 | 1918610 | 20.0 |