LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090718\
Data File : BF108857.D
Acq On : 7 Sep 2018 13:44
Operator : JU/SJ
Sample : J4741-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOC2-03-B

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-BF090518.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 | 4.284 | 326 | 331 | 339 | rBV | 1441370 | 1680831 | 31.16% | 3.766% |
| 2 | 4.925 | 435 | 440 | 452 | rVB | 1153034 | 1368370 | 25.36% | 3.066% |
| 3 | 5.343 | 506 | 511 | 514 | rBV | 3761659 | 3607856 | 66.87% | 8.083% |
| 4 | 6.372 | 680 | 686 | 688 | rBV | 3621162 | 3884649 | 72.00% | 8.703% |
| 5 | 6.501 | 704 | 708 | 712 | rBV | 3799420 | 3801615 | 70.47% | 8.517% |
| 6 | 6.737 | 744 | 748 | 751 | rBV | 1667487 | 1303997 | 24.17% | 2.921% |
| 7 | 6.895 | 770 | 775 | 778 | rBV | 4542040 | 3915443 | 72.58% | 8.772% |
| 8 | 7.295 | 838 | 843 | 846 | rBV | 3487442 | 3106771 | 57.59% | 6.960% |
| 9 | 8.019 | 962 | 966 | 969 | rBV | 1879727 | 1661888 | 30.80% | 3.723% |
| 10 | 9.095 | 1144 | 1149 | 1152 | rBV | 6253170 | 5395007 | 100.00% | 12.086% |
| 11 | 9.483 | 1211 | 1215 | 1218 | rBV | 372666 | 285981 | 5.30% | 0.641% |
| 12 | 9.766 | 1259 | 1263 | 1267 | rBV | 2194282 | 1759863 | 32.62% | 3.943% |
| 13 | 10.548 | 1392 | 1396 | 1399 | rBV | 2199890 | 1902813 | 35.27% | 4.263% |
| 14 | 11.242 | 1510 | 1514 | 1517 | rBV | 1966862 | 1575198 | 29.20% | 3.529% |
| 15 | 11.777 | 1601 | 1605 | 1609 | rBV4 | 57865 | 68541 | 1.27% | 0.154% |
| 16 | 12.448 | 1716 | 1719 | 1723 | rVB | 104915 | 90552 | 1.68% | 0.203% |
| 17 | 12.671 | 1751 | 1757 | 1760 | rBV2 | 103318 | 150746 | 2.79% | 0.338% |
| 18 | 12.824 | 1779 | 1783 | 1787 | rBV | 4705487 | 4532255 | 84.01% | 10.154% |
| 19 | 13.736 | 1935 | 1938 | 1945 | rVB3 | 126071 | 177617 | 3.29% | 0.398% |
| 20 | 13.865 | 1956 | 1960 | 1963 | rBV | 1866460 | 1635896 | 30.32% | 3.665% |
| 21 | 14.360 | 2042 | 2044 | 2049 | rBV | 97773 | 137822 | 2.55% | 0.309% |
| 22 | 14.630 | 2087 | 2090 | 2092 | rBV | 255786 | 257899 | 4.78% | 0.578% |
| 23 | 14.660 | 2092 | 2095 | 2100 | rVB2 | 139507 | 187303 | 3.47% | 0.420% |
| 24 | 14.977 | 2146 | 2149 | 2155 | rVB | 257104 | 275670 | 5.11% | 0.618% |
| 25 | 15.277 | 2195 | 2200 | 2203 | rVB | 1072169 | 1285289 | 23.82% | 2.879% |
| 26 | 15.336 | 2207 | 2210 | 2214 | rVB | 234209 | 289299 | 5.36% | 0.648% |
| 27 | 15.742 | 2276 | 2279 | 2283 | rBV | 251144 | 297605 | 5.52% | 0.667% |

Sum of corrected areas: 44636776

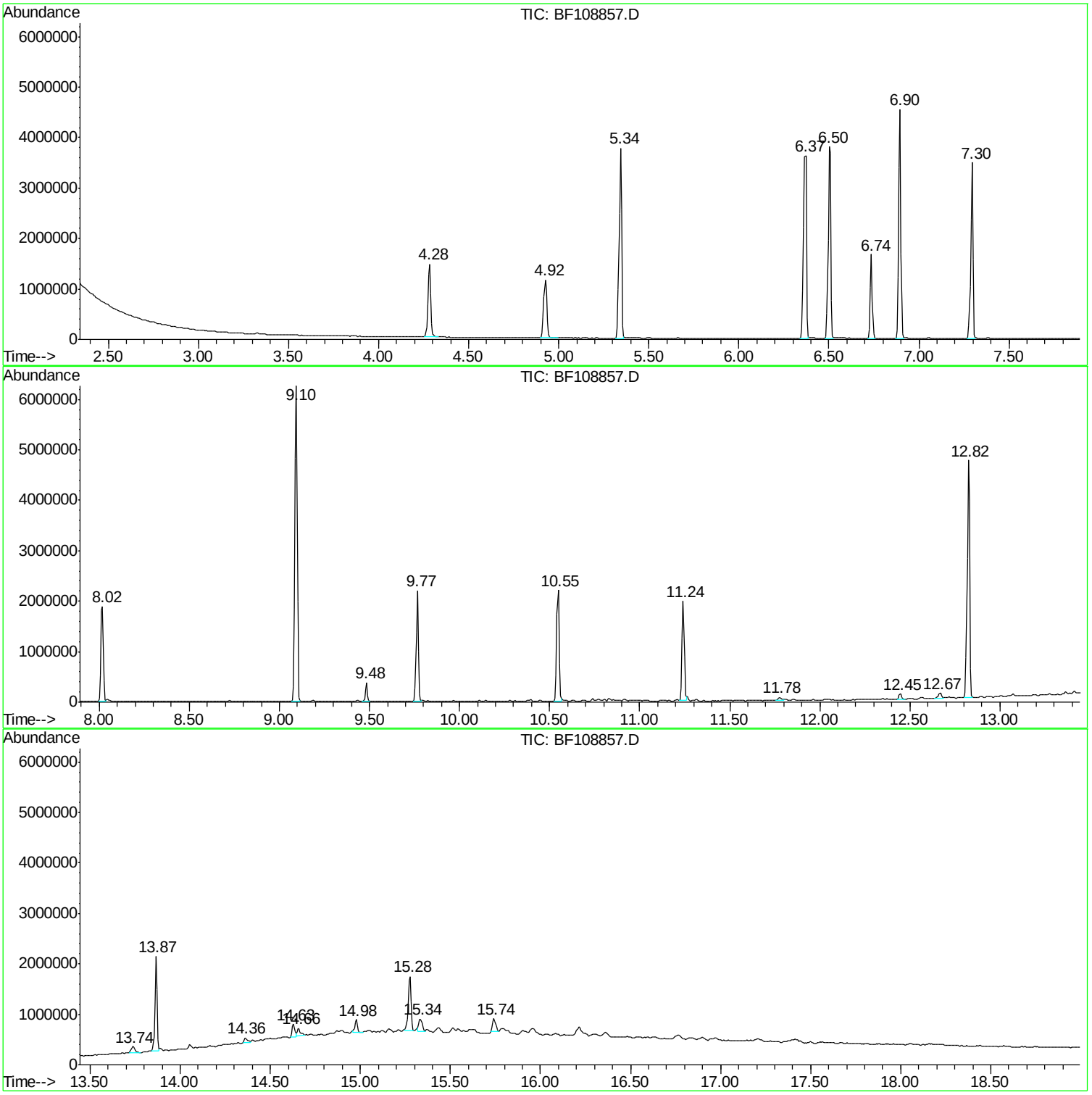
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090718\
Data File : BF108857.D
Acq On : 7 Sep 2018 13:44
Operator : JU/SJ
Sample : J4741-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOC2-03-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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\BF090718\
Data File : BF108857.D
Acq On : 7 Sep 2018 13:44
Operator : JU/SJ
Sample : J4741-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOC2-03-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

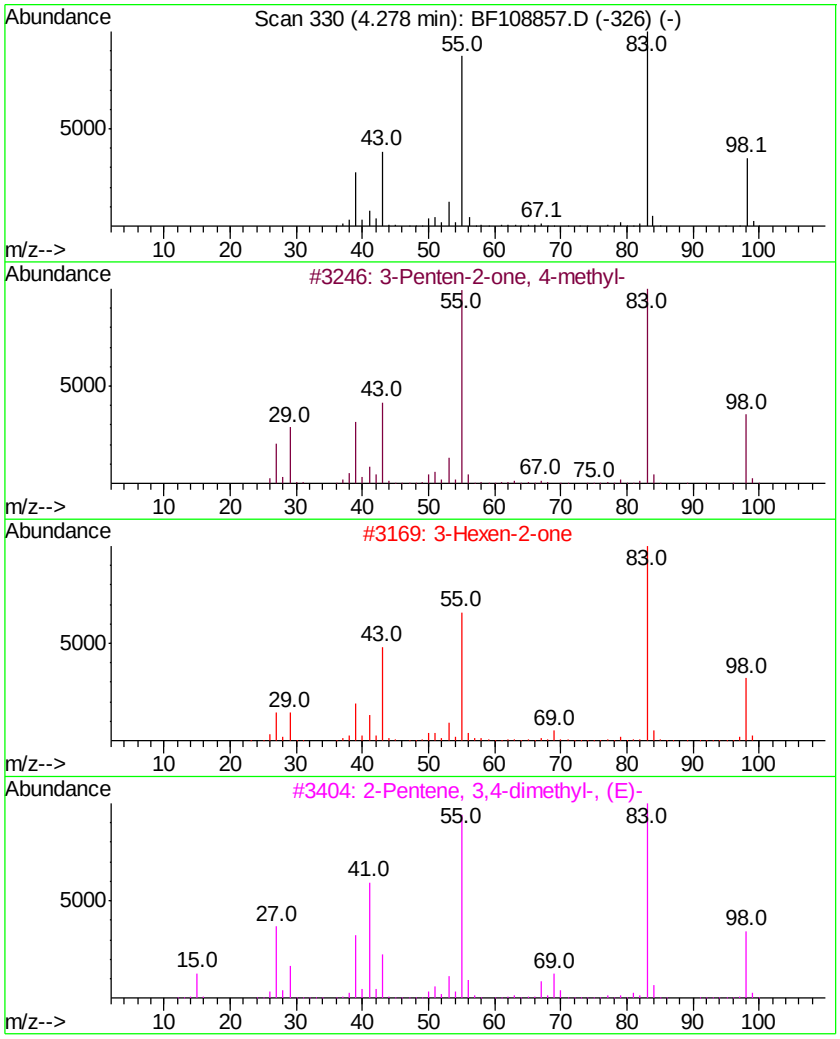
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

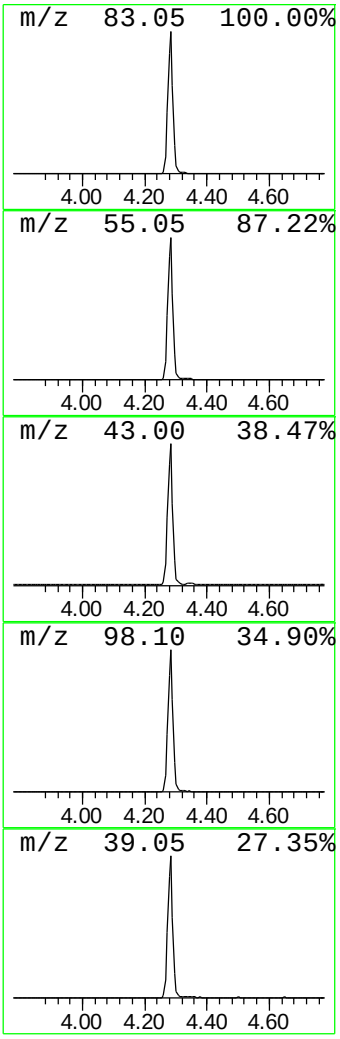
**********

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.28 | 25.78 ng | 1680830 | 1,4-Dichlorobenzene-d4 | 6.74 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Penten-2-one, 4-methyl- | 98 | C6H10O | 000141-79-7 | 94 |
| 2 | 3-Hexen-2-one | 98 | C6H10O | 000763-93-9 | 87 |
| 3 | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14 | 004914-92-5 | 86 |
| 4 | 2-Pentene, 2,4-dimethyl- | 98 | C7H14 | 000625-65-0 | 80 |
| 5 | 2-Pentene, 3,4-dimethyl-, (Z)- | 98 | C7H14 | 004914-91-4 | 80 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090718\
Data File : BF108857.D
Acq On : 7 Sep 2018 13:44
Operator : JU/SJ
Sample : J4741-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOC2-03-B

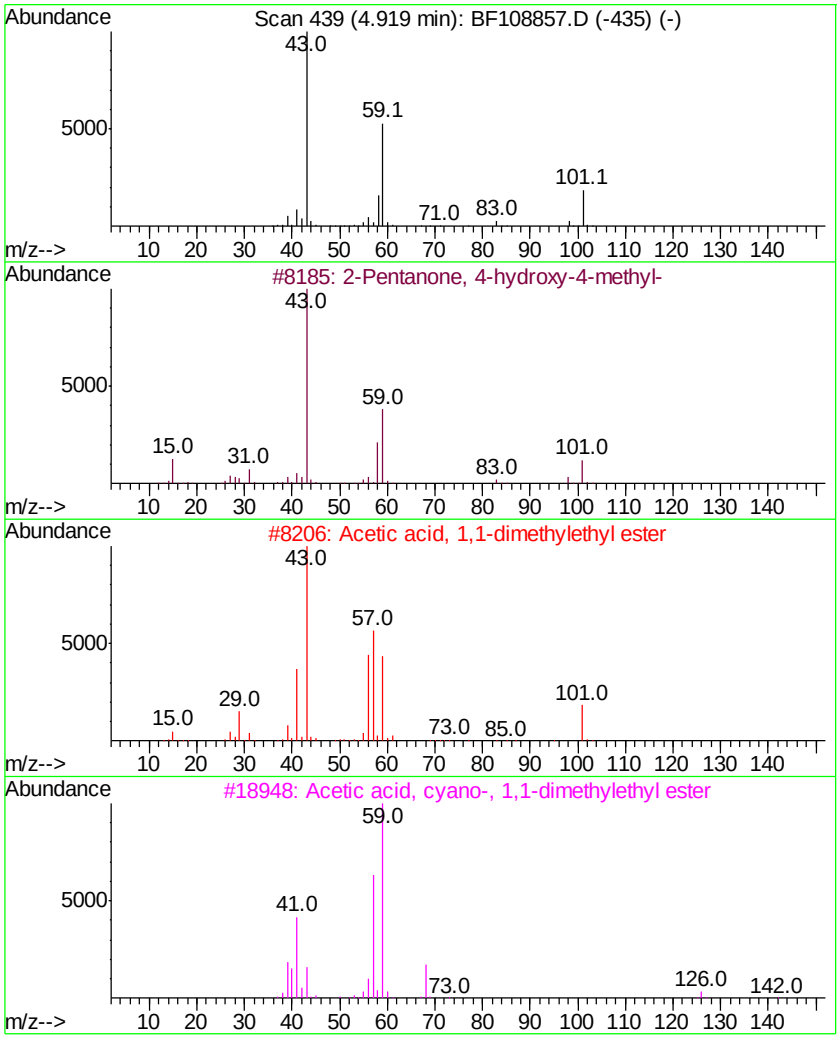
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

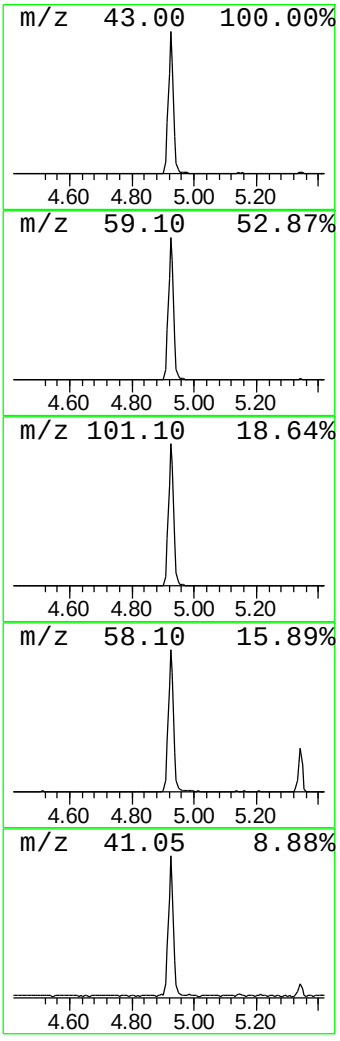
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.92 | 20.99 ng | 1368370 | 1,4-Dichlorobenzene-d4 | 6.74 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 59 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39 |
| 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\BF090718\
Data File : BF108857.D
Acq On : 7 Sep 2018 13:44
Operator : JU/SJ
Sample : J4741-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOC2-03-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

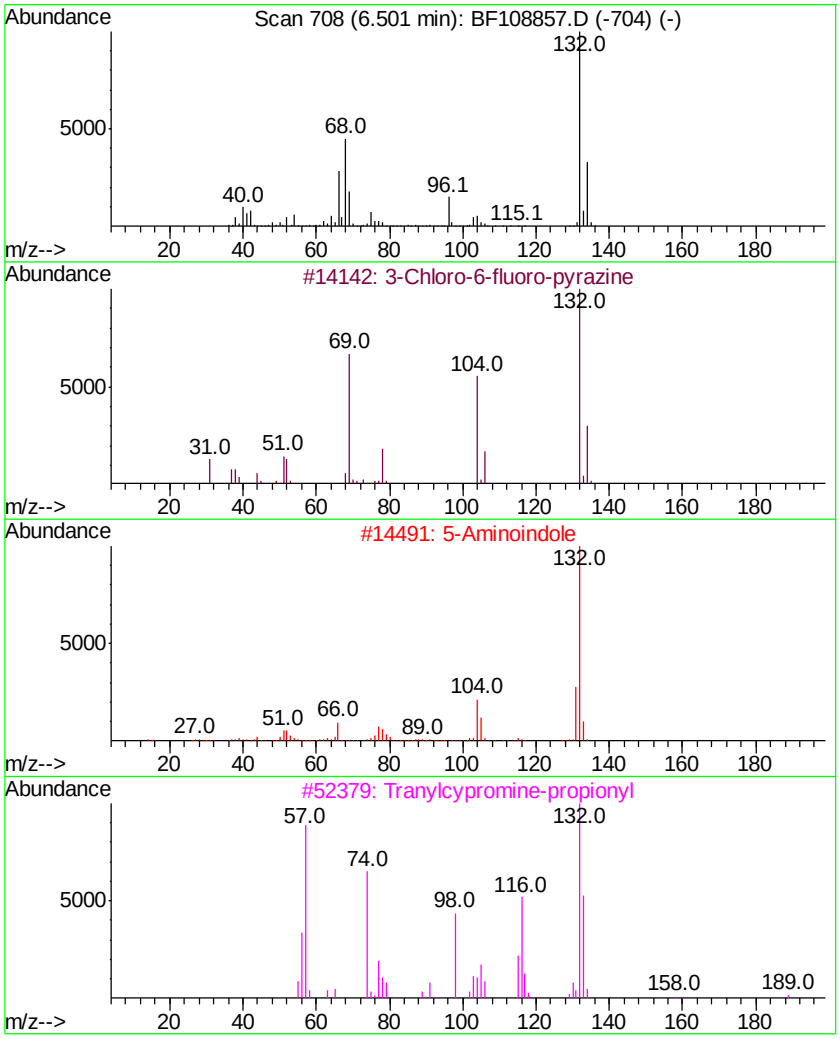
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

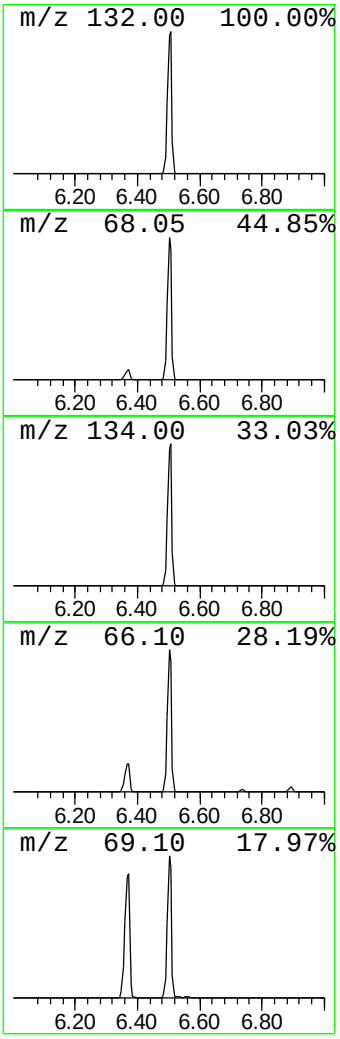
**********

Peak Number 3 unknown6.50 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.50 | 58.31 ng | 3801620 | 1,4-Dichlorobenzene-d4 | 6.74 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 5 | Benzene, 1-ethenyl-3,5-dimethyl- | 132 | C10H12 | 005379-20-4 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090718\
Data File : BF108857.D
Acq On : 7 Sep 2018 13:44
Operator : JU/SJ
Sample : J4741-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOC2-03-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

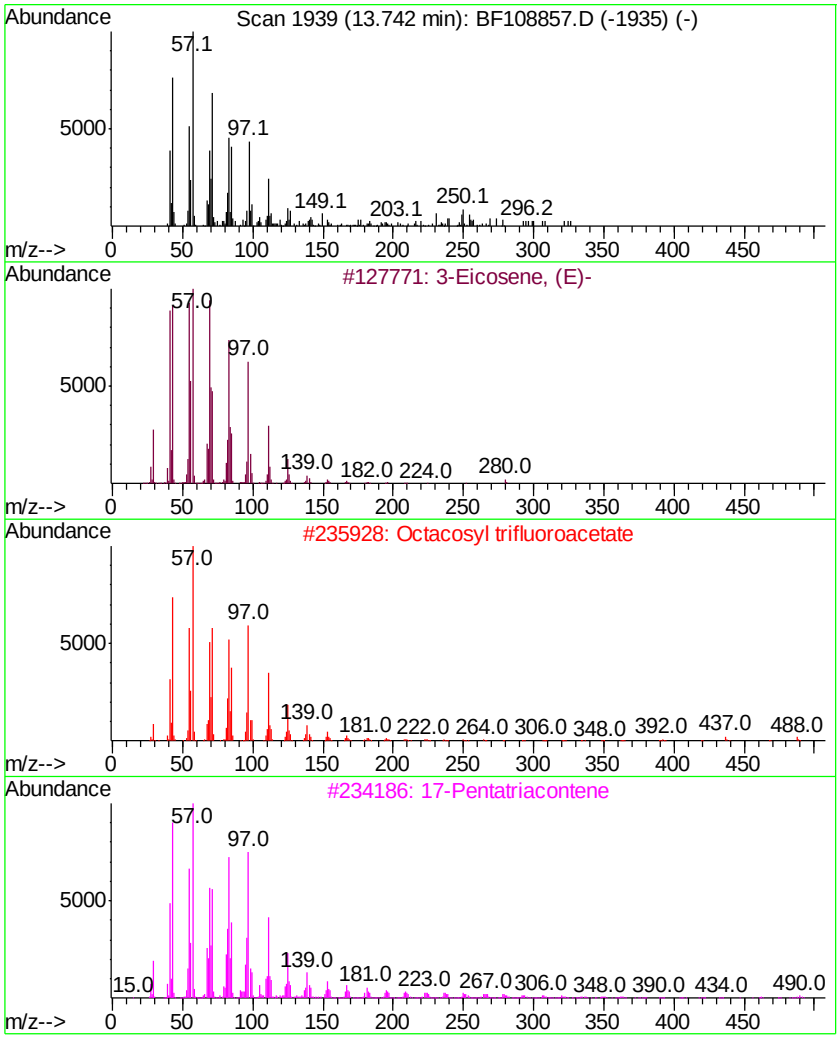
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

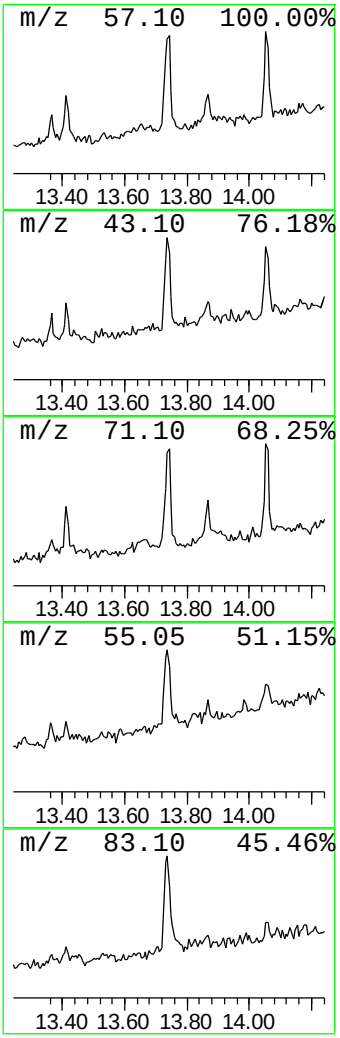
**********

Peak Number 5 3-Eicosene, (E)- Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.74 | 2.17 ng | 177617 | Chrysene-d12 | 13.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Eicosene, (E)- | 280 | C20H40 | 074685-33-9 | 95 |
| 2 | Octacosyl trifluoroacetate | 506 | C30H57F3O2 | 1000351-74-9 | 90 |
| 3 | 17-Pentatriacontene | 491 | C35H70 | 006971-40-0 | 90 |
| 4 | Nonadecyl pentafluoropropionate | 430 | C22H39F5O2 | 1000351-88-8 | 90 |
| 5 | 3-Octadecene, (E)- | 252 | C18H36 | 007206-19-1 | 87 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090718\
Data File : BF108857.D
Acq On : 7 Sep 2018 13:44
Operator : JU/SJ
Sample : J4741-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOC2-03-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

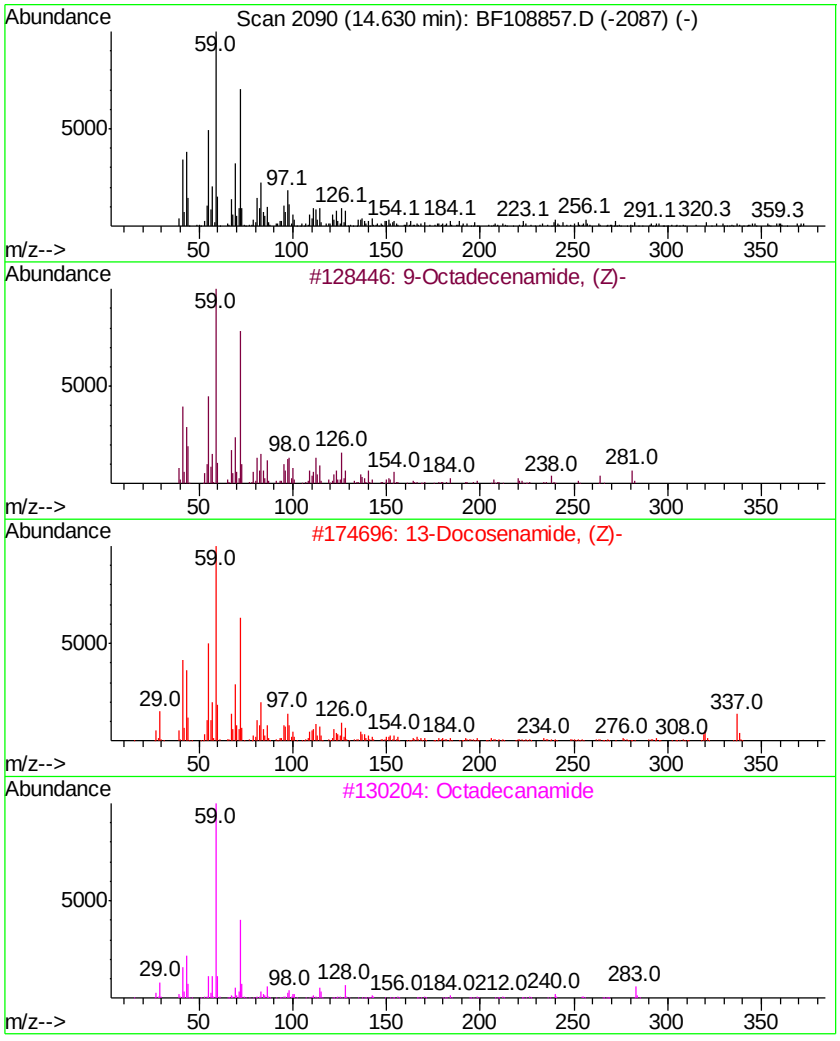
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

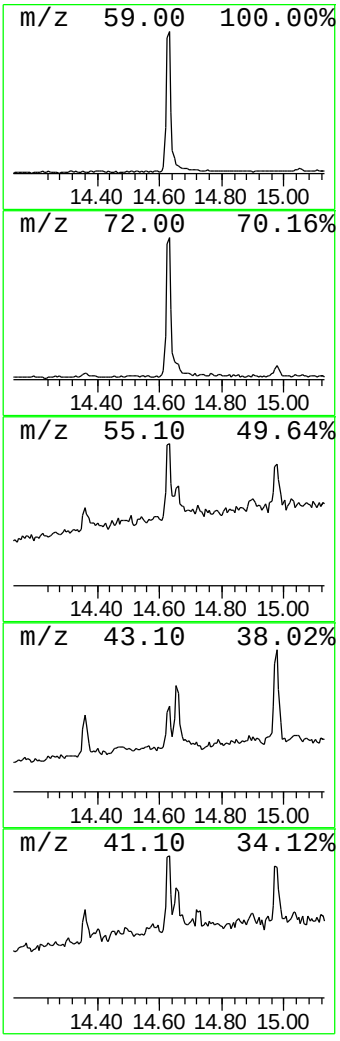
**********

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.63 | 4.01 ng | 257899 | Perylene-d12 | 15.28 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9-Octadecenamide, (Z)- | 281 | C18H35NO | 000301-02-0 | 94 |
| 2 | 13-Docosenamide, (Z)- | 337 | C22H43NO | 000112-84-5 | 81 |
| 3 | Octadecanamide | 283 | C18H37NO | 000124-26-5 | 53 |
| 4 | 7-Nonenamide | 155 | C9H17NO | 090949-53-4 | 50 |
| 5 | 3-Tridecanol | 200 | C13H28O | 010289-68-6 | 47 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090718\
Data File : BF108857.D
Acq On : 7 Sep 2018 13:44
Operator : JU/SJ
Sample : J4741-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOC2-03-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

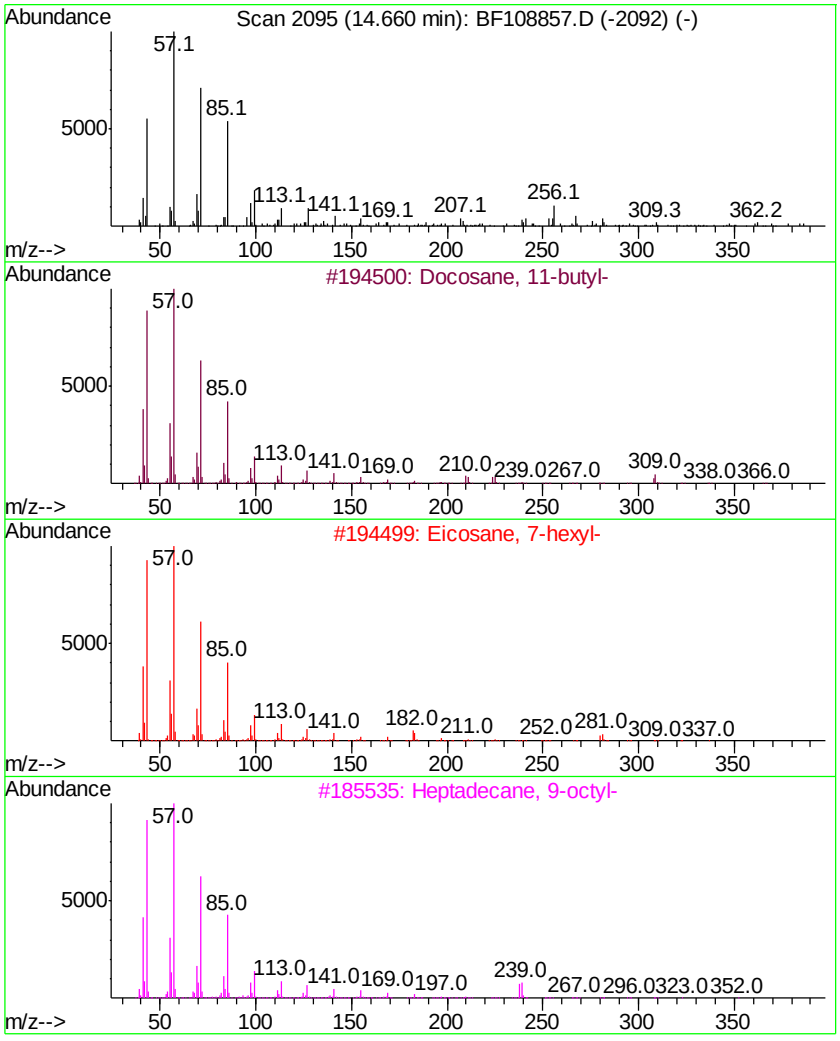
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

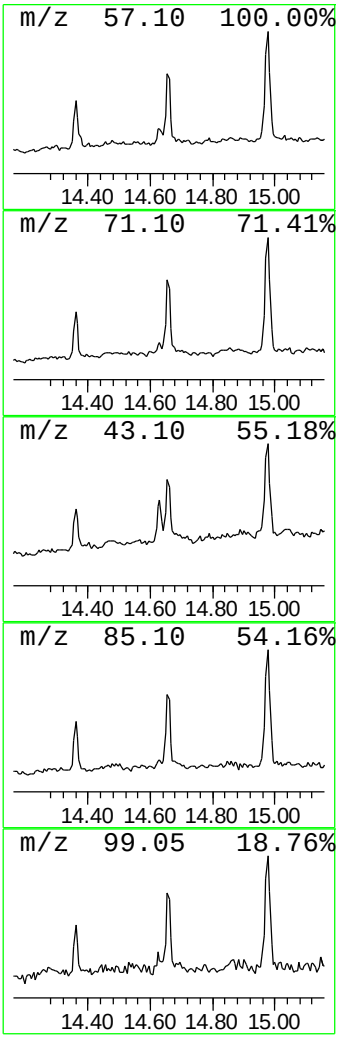
**********

Peak Number 7 Docosane, 11-butyl- Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.66 | 2.91 ng | 187303 | Perylene-d12 | 15.28 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Docosane, 11-butyl- | 366 | C26H54 | 013475-76-8 | 87 |
| 2 | Eicosane, 7-hexyl- | 366 | C26H54 | 055333-99-8 | 86 |
| 3 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 80 |
| 4 | Tetracosane | 338 | C24H50 | 000646-31-1 | 72 |
| 5 | Pentadecane | 212 | C15H32 | 000629-62-9 | 59 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090718\
Data File : BF108857.D
Acq On : 7 Sep 2018 13:44
Operator : JU/SJ
Sample : J4741-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOC2-03-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

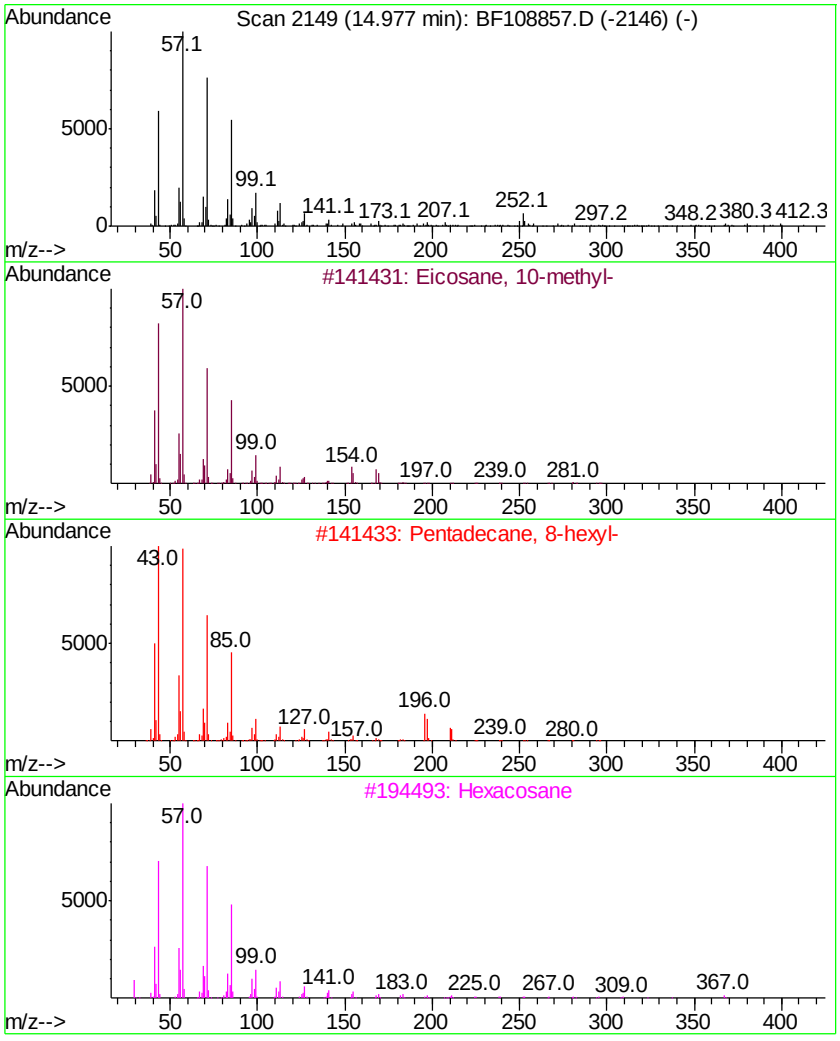
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

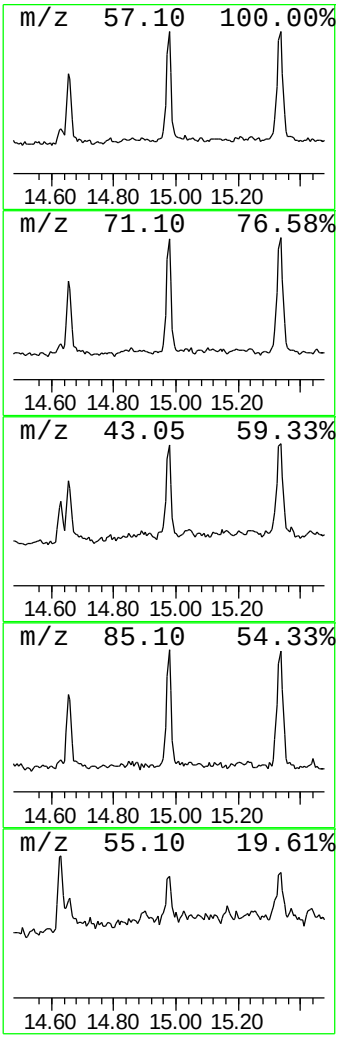
**********

Peak Number 8 Eicosane, 10-methyl- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.98 | 4.29 ng | 275670 | Perylene-d12 | 15.28 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane, 10-methyl- | 296 | C21H44 | 054833-23-7 | 93 |
| 2 | Pentadecane, 8-hexyl- | 296 | C21H44 | 013475-75-7 | 90 |
| 3 | Hexacosane | 366 | C26H54 | 000630-01-3 | 87 |
| 4 | Decane, 3,8-dimethyl- | 170 | C12H26 | 017312-55-9 | 87 |
| 5 | Octadecane, 1-iodo- | 380 | C18H37I | 000629-93-6 | 86 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090718\
Data File : BF108857.D
Acq On : 7 Sep 2018 13:44
Operator : JU/SJ
Sample : J4741-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOC2-03-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

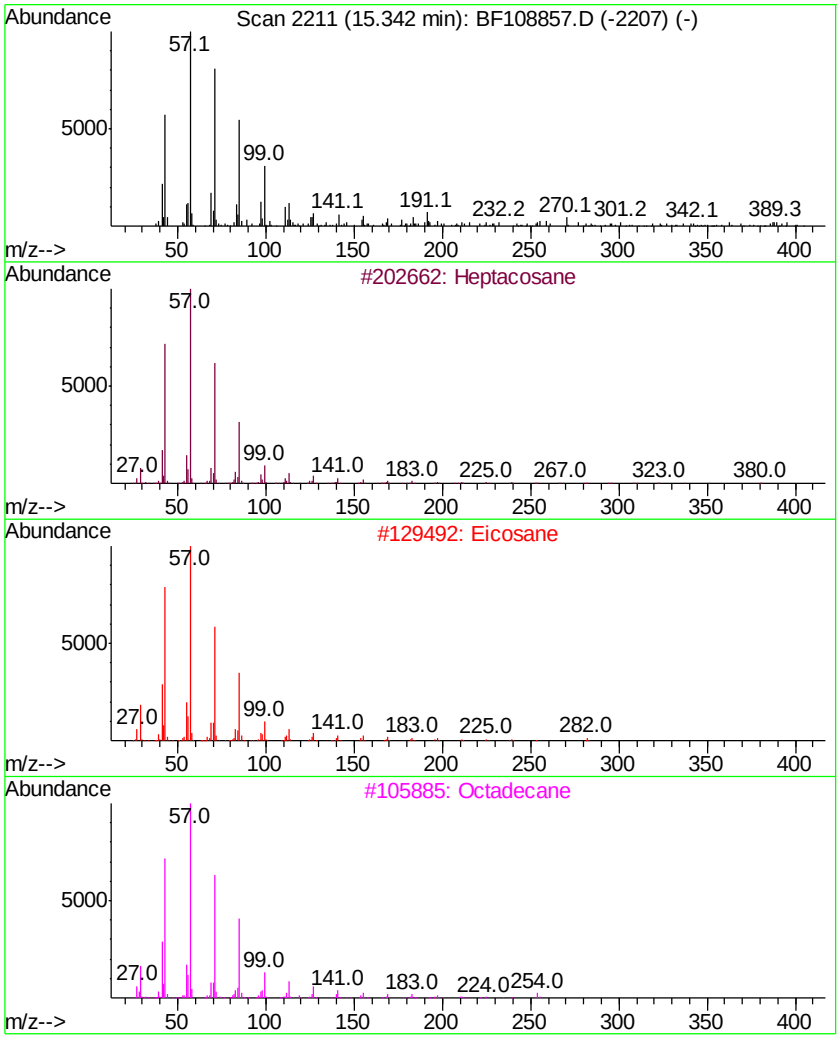
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

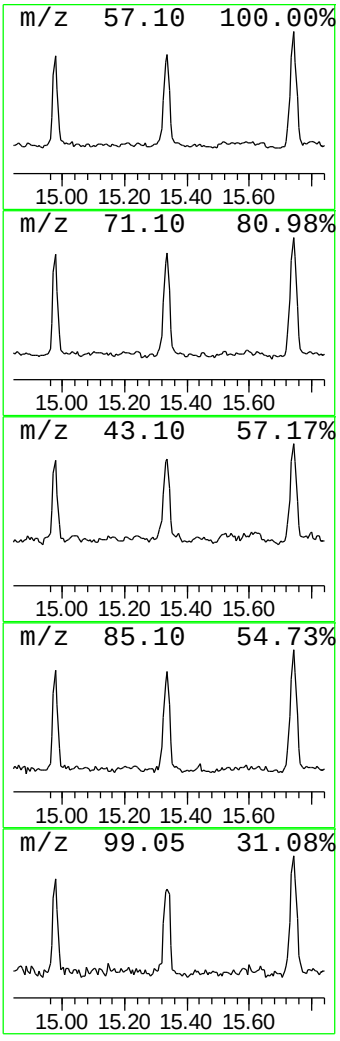
**********

Peak Number 9 Heptacosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.34 | 4.50 ng | 289299 | Perylene-d12 | 15.28 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptacosane | 380 | C27H56 | 000593-49-7 | 93 |
| 2 | Eicosane | 282 | C20H42 | 000112-95-8 | 87 |
| 3 | Octadecane | 254 | C18H38 | 000593-45-3 | 87 |
| 4 | Tetracosane | 338 | C24H50 | 000646-31-1 | 87 |
| 5 | Triacontane | 422 | C30H62 | 000638-68-6 | 87 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090718\
Data File : BF108857.D
Acq On : 7 Sep 2018 13:44
Operator : JU/SJ
Sample : J4741-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOC2-03-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

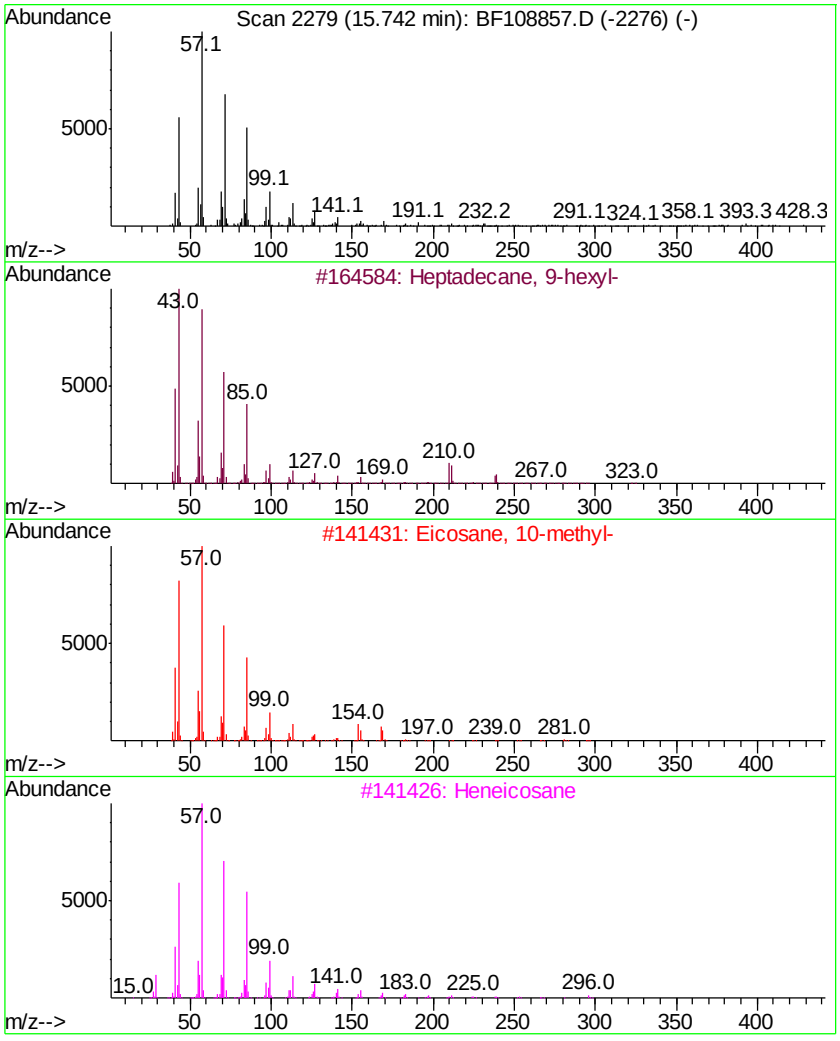
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

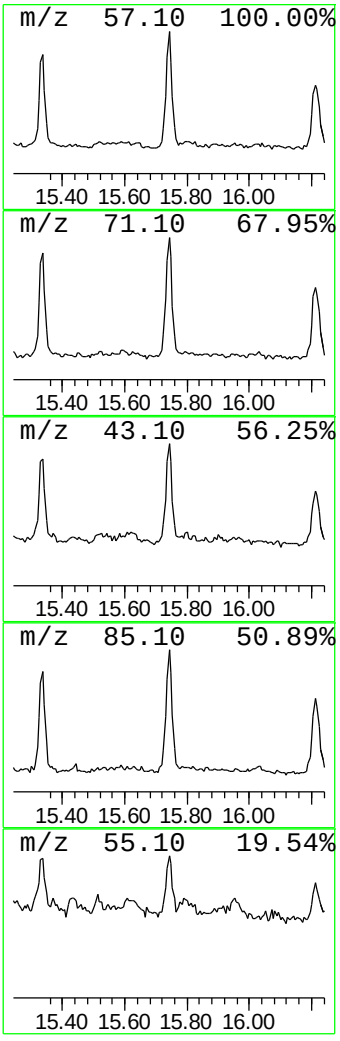
**********

Peak Number 10 Heptadecane, 9-hexyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.74 | 4.63 ng | 297605 | Perylene-d12 | 15.28 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane, 9-hexyl- | 324 | C23H48 | 055124-79-3 | 93 |
| 2 | Eicosane, 10-methyl- | 296 | C21H44 | 054833-23-7 | 90 |
| 3 | Heneicosane | 296 | C21H44 | 000629-94-7 | 87 |
| 4 | Pentadecane | 212 | C15H32 | 000629-62-9 | 87 |
| 5 | Tetracosane | 338 | C24H50 | 000646-31-1 | 87 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090718\
Data File : BF108857.D
Acq On : 7 Sep 2018 13:44
Operator : JU/SJ
Sample : J4741-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOC2-03-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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 |
| 3-Penten-2-one, 4... | 4.28 | 25.8 | ng | 1680830 | 1 | 6.74 | 1304000 | 20.0 |
| 2-Pentanone, 4-hy... | 4.92 | 21.0 | ng | 1368370 | 1 | 6.74 | 1304000 | 20.0 |
| unknown6.50 | 6.50 | 58.3 | ng | 3801620 | 1 | 6.74 | 1304000 | 20.0 |
| 3-Eicosene, (E)- | 13.74 | 2.2 | ng | 177617 | 5 | 13.87 | 1635900 | 20.0 |
| 9-Octadecenamide,... | 14.63 | 4.0 | ng | 257899 | 6 | 15.28 | 1285290 | 20.0 |
| Docosane, 11-butyl- | 14.66 | 2.9 | ng | 187303 | 6 | 15.28 | 1285290 | 20.0 |
| Eicosane, 10-methyl- | 14.98 | 4.3 | ng | 275670 | 6 | 15.28 | 1285290 | 20.0 |
| Heptacosane | 15.34 | 4.5 | ng | 289299 | 6 | 15.28 | 1285290 | 20.0 |
| Heptadecane, 9-he... | 15.74 | 4.6 | ng | 297605 | 6 | 15.28 | 1285290 | 20.0 |