LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110642.D
Acq On : 9 Nov 2018 22:03
Operator : JU/SJ
Sample : J5813-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-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-BF110818.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 | 2.246 | 22 | 27 | 41 | rVB | 269558 | 352487 | 18.62% | 2.059% |
| 2 | 5.181 | 522 | 526 | 536 | rBV | 46798 | 67802 | 3.58% | 0.396% |
| 3 | 5.563 | 587 | 591 | 605 | rBV | 1673473 | 1642014 | 86.74% | 9.590% |
| 4 | 6.569 | 757 | 762 | 767 | rBV | 1716604 | 1855708 | 98.02% | 10.839% |
| 5 | 6.610 | 767 | 769 | 782 | rVB | 36727 | 50797 | 2.68% | 0.297% |
| 6 | 6.716 | 782 | 787 | 790 | rBV | 1920315 | 1815456 | 95.90% | 10.603% |
| 7 | 6.945 | 822 | 826 | 832 | rBV | 556281 | 498523 | 26.33% | 2.912% |
| 8 | 7.098 | 848 | 852 | 863 | rBV | 1546941 | 1347581 | 71.18% | 7.871% |
| 9 | 7.510 | 917 | 922 | 937 | rBV | 1232138 | 1149267 | 60.71% | 6.712% |
| 10 | 8.228 | 1040 | 1044 | 1056 | rBV | 692526 | 672211 | 35.51% | 3.926% |
| 11 | 8.310 | 1056 | 1058 | 1071 | rVB2 | 13201 | 22642 | 1.20% | 0.132% |
| 12 | 9.298 | 1222 | 1226 | 1229 | rBV | 2318730 | 1893106 | 100.00% | 11.057% |
| 13 | 9.692 | 1289 | 1293 | 1299 | rBV | 243208 | 222590 | 11.76% | 1.300% |
| 14 | 9.986 | 1339 | 1343 | 1355 | rVB | 759888 | 715246 | 37.78% | 4.178% |
| 15 | 10.774 | 1474 | 1477 | 1490 | rBV | 1011459 | 997425 | 52.69% | 5.826% |
| 16 | 11.480 | 1593 | 1597 | 1599 | rBV | 632323 | 581039 | 30.69% | 3.394% |
| 17 | 11.504 | 1599 | 1601 | 1604 | rVB | 80637 | 71882 | 3.80% | 0.420% |
| 18 | 11.980 | 1680 | 1682 | 1686 | rBV | 78707 | 76609 | 4.05% | 0.447% |
| 19 | 12.698 | 1800 | 1804 | 1809 | rBV | 150072 | 141119 | 7.45% | 0.824% |
| 20 | 12.927 | 1837 | 1843 | 1849 | rVB | 125243 | 145025 | 7.66% | 0.847% |
| 21 | 13.057 | 1861 | 1865 | 1869 | rBV | 1281440 | 1213017 | 64.08% | 7.085% |
| 22 | 13.610 | 1956 | 1959 | 1964 | rBV7 | 16100 | 22519 | 1.19% | 0.132% |
| 23 | 13.768 | 1983 | 1986 | 1989 | rBV2 | 16445 | 23347 | 1.23% | 0.136% |
| 24 | 13.939 | 2011 | 2015 | 2020 | rBV3 | 116860 | 150233 | 7.94% | 0.877% |
| 25 | 14.127 | 2043 | 2047 | 2050 | rBV | 511291 | 506854 | 26.77% | 2.960% |
| 26 | 14.157 | 2050 | 2052 | 2056 | rVB | 52453 | 45792 | 2.42% | 0.267% |
| 27 | 14.562 | 2118 | 2121 | 2127 | rBV4 | 43548 | 69779 | 3.69% | 0.408% |
| 28 | 14.874 | 2172 | 2174 | 2178 | rVB | 47703 | 47063 | 2.49% | 0.275% |
| 29 | 15.033 | 2198 | 2201 | 2204 | rBV2 | 68143 | 64901 | 3.43% | 0.379% |
| 30 | 15.204 | 2227 | 2230 | 2232 | rBV | 50214 | 64576 | 3.41% | 0.377% |
| 31 | 15.227 | 2232 | 2234 | 2237 | rVB | 95516 | 91949 | 4.86% | 0.537% |
| 32 | 15.621 | 2299 | 2301 | 2303 | rBV2 | 41127 | 46794 | 2.47% | 0.273% |
| 33 | 15.656 | 2303 | 2307 | 2311 | rVB | 256012 | 322057 | 17.01% | 1.881% |
| 34 | 16.080 | 2375 | 2379 | 2384 | rVB | 87284 | 133903 | 7.07% | 0.782% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110642.D
Acq On : 9 Nov 2018 22:03
Operator : JU/SJ
Sample : J5813-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TS-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-BF110818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 17121313

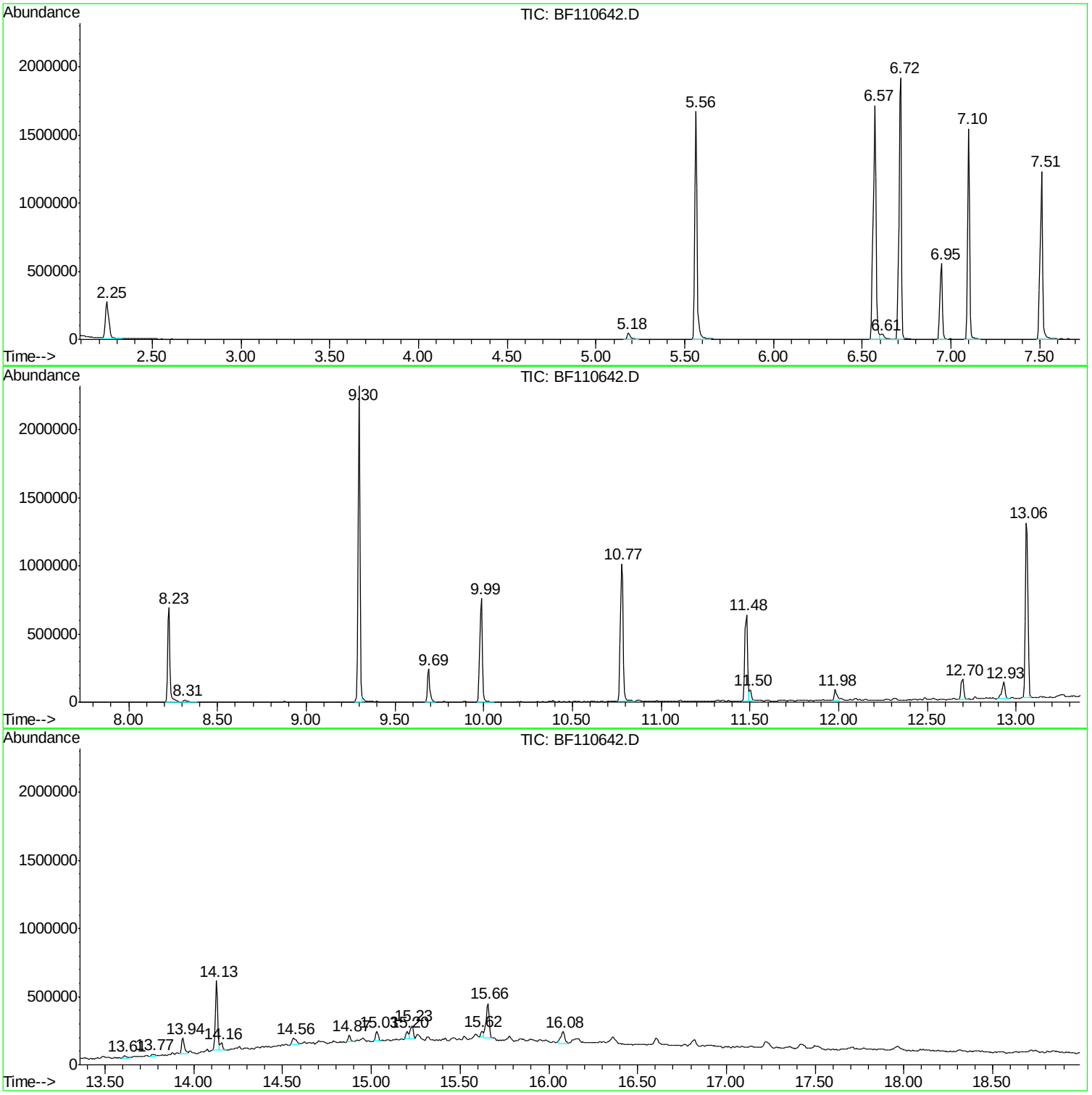
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110642.D
Acq On : 9 Nov 2018 22:03
Operator : JU/SJ
Sample : J5813-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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\BF110918\
Data File : BF110642.D
Acq On : 9 Nov 2018 22:03
Operator : JU/SJ
Sample : J5813-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

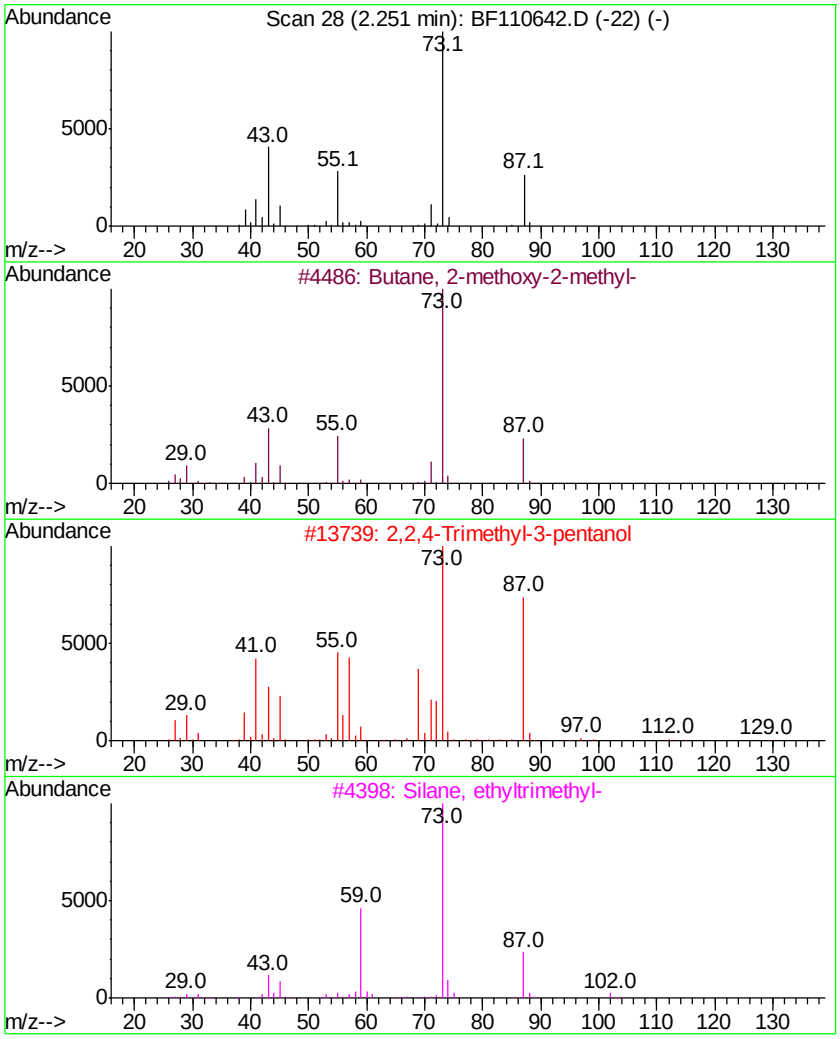
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

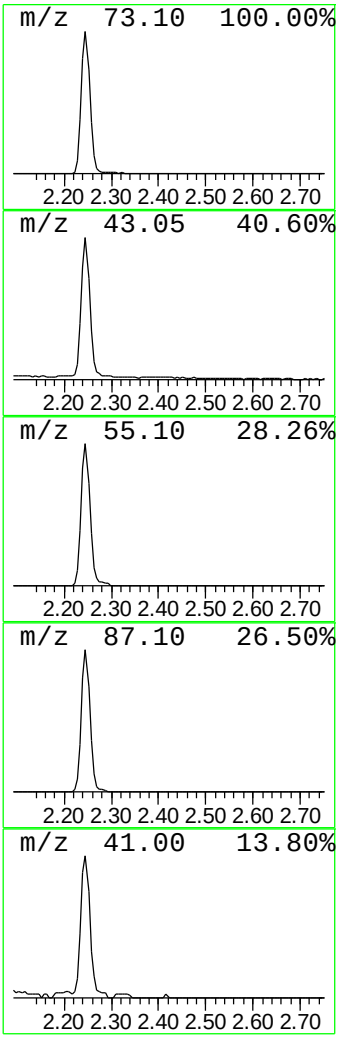
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.25 | 14.14 ng | 352487 | 1,4-Dichlorobenzene-d4 | 6.95 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 83 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 39 |
| 3 | Silane, ethyltrimethyl- | 102 | C5H14Si | 003439-38-1 | 33 |
| 4 | Acetamide, N-ethyl- | 87 | C4H9NO | 000625-50-3 | 12 |
| 5 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 12 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110642.D
Acq On : 9 Nov 2018 22:03
Operator : JU/SJ
Sample : J5813-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

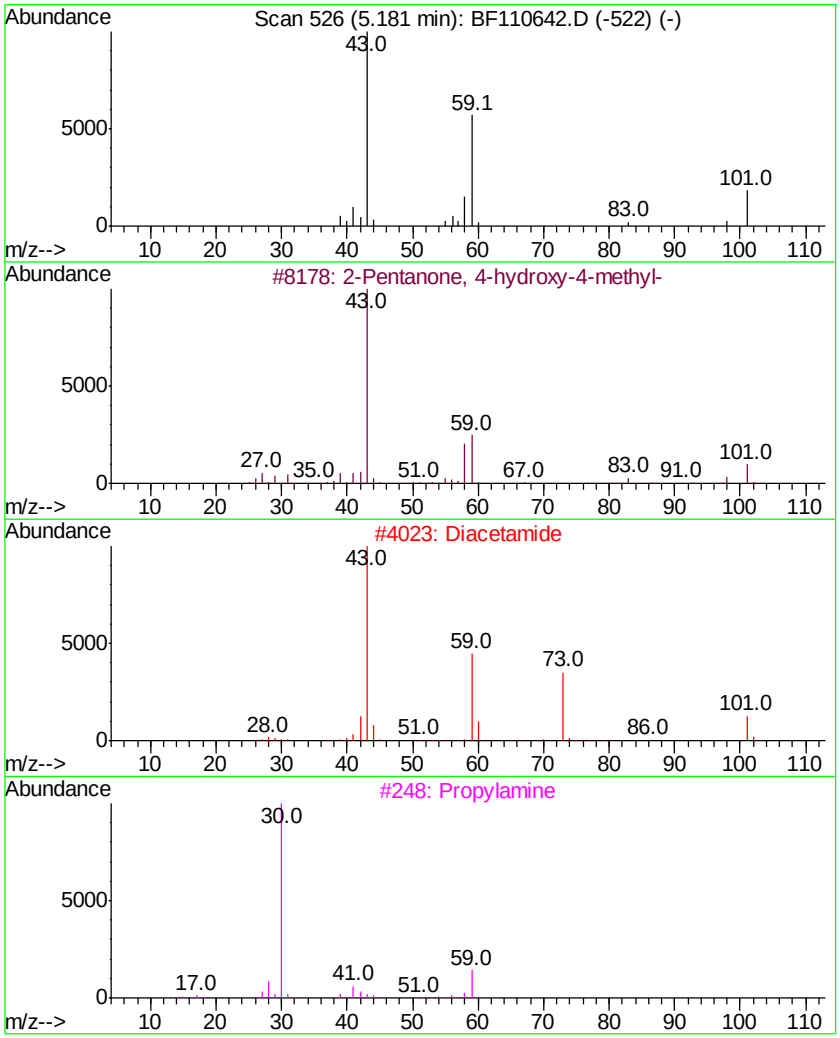
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

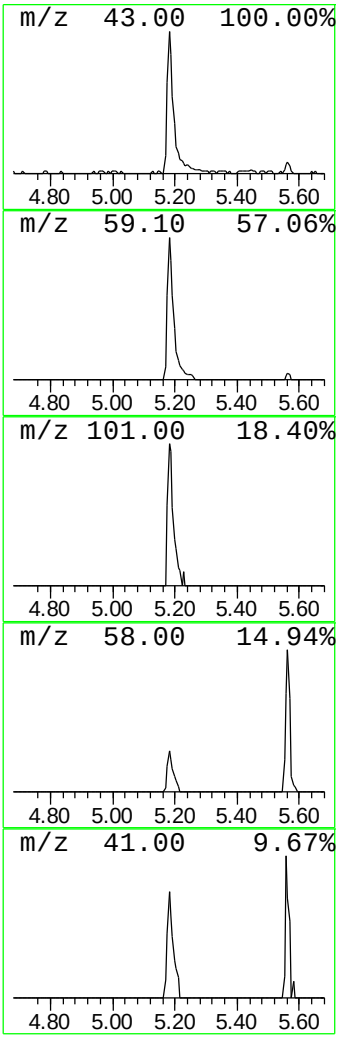
**********

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.18 | 2.72 ng | 67802 | 1,4-Dichlorobenzene-d4 | 6.95 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | Diacetamide | 101 | C4H7NO2 | 000625-77-4 | 9 |
| 3 | Propylamine | 59 | C3H9N | 000107-10-8 | 9 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 5 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 9 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110642.D
Acq On : 9 Nov 2018 22:03
Operator : JU/SJ
Sample : J5813-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

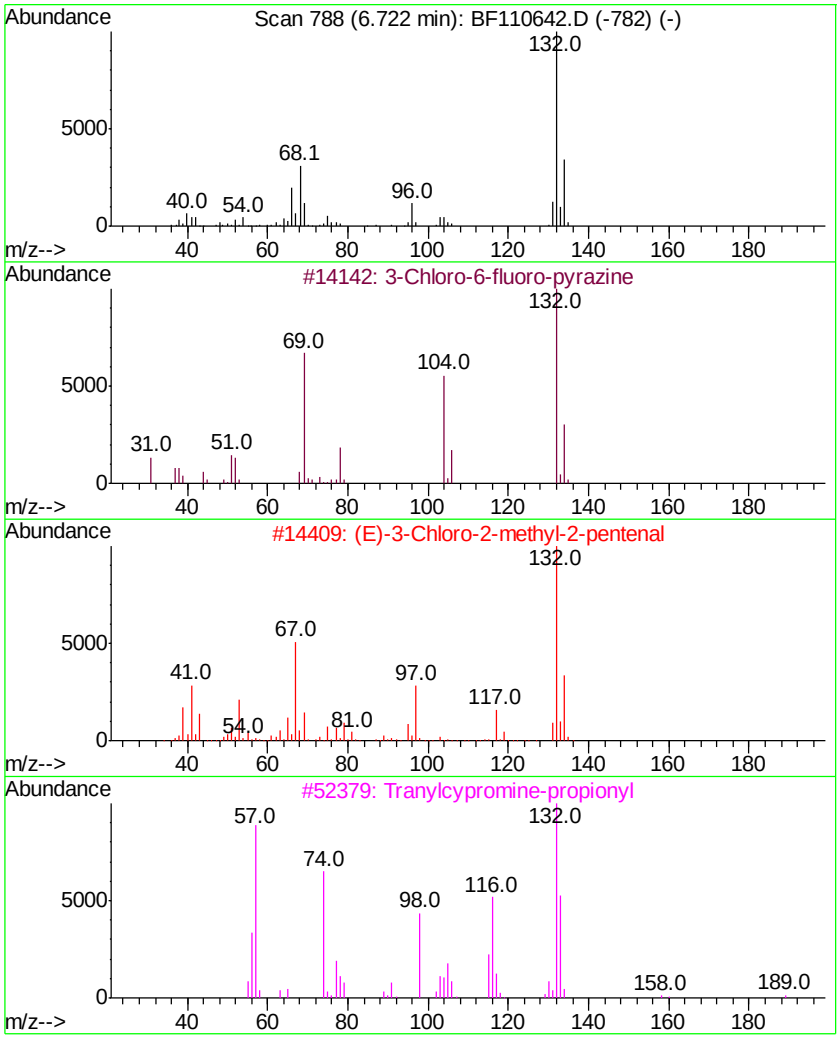
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

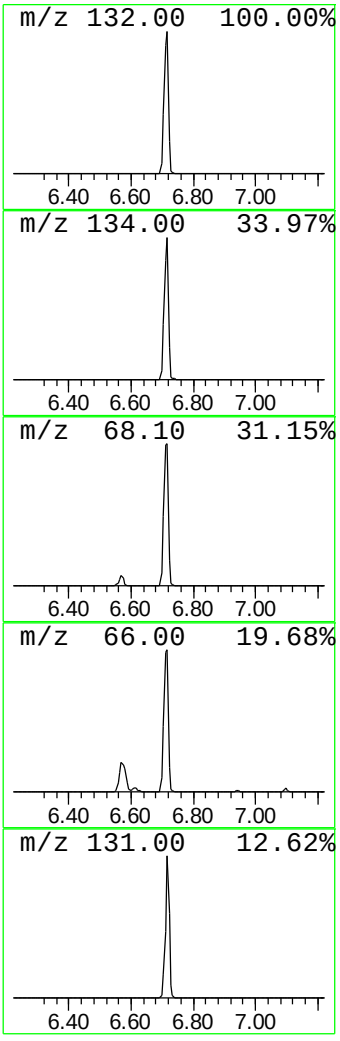
**********

Peak Number 3 unknown6.72 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.72 | 72.83 ng | 1815460 | 1,4-Dichlorobenzene-d4 | 6.95 |

| 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 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 16 |
| 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\BF110918\
Data File : BF110642.D
Acq On : 9 Nov 2018 22:03
Operator : JU/SJ
Sample : J5813-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

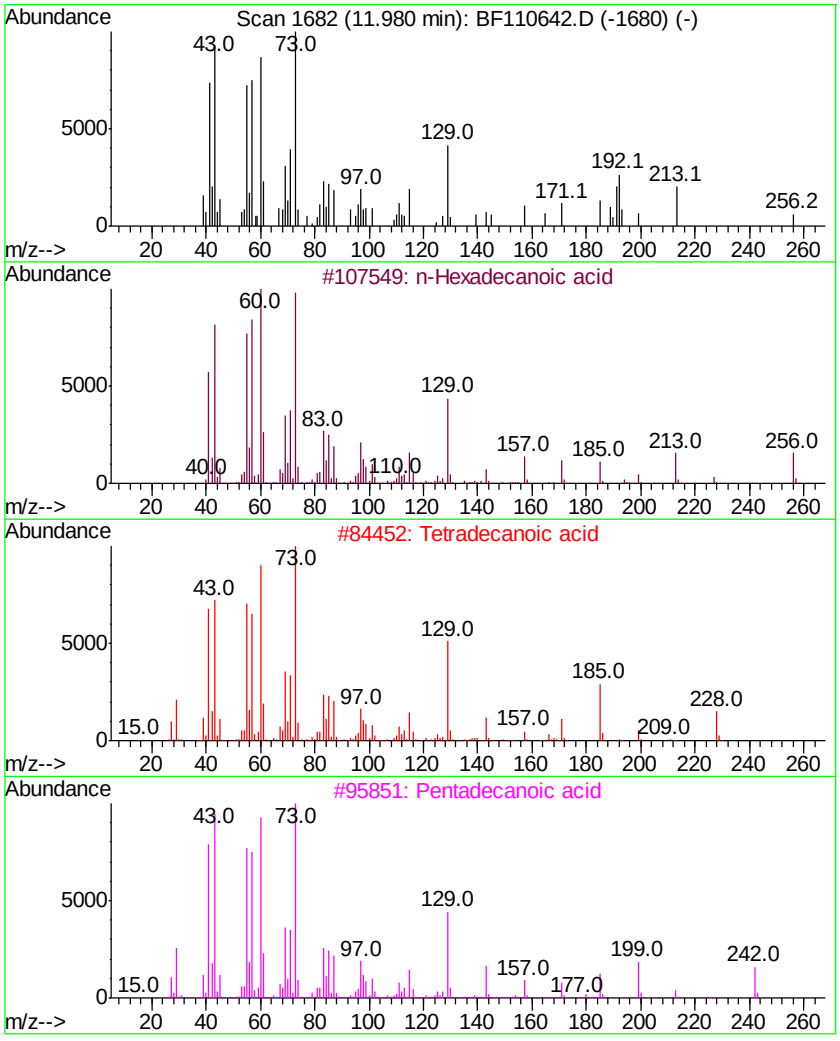
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

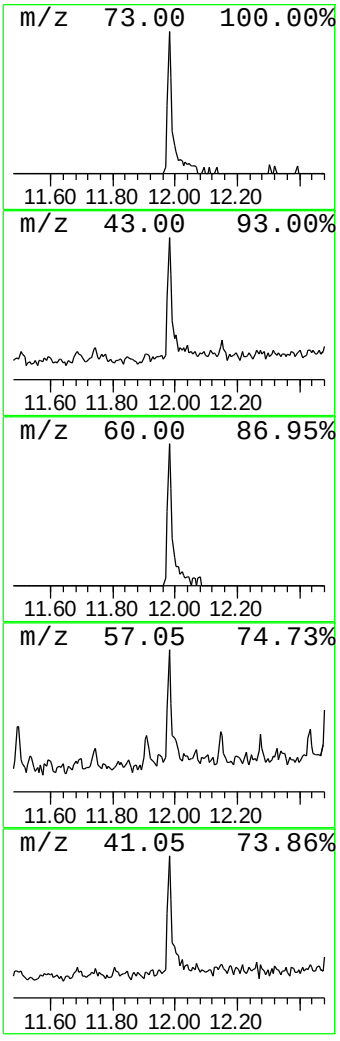
**********

Peak Number 5 n-Hexadecanoic acid Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.98 | 2.64 ng | 76609 | Phenanthrene-d10 | 11.48 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 96 |
| 2 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 64 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 64 |
| 4 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 58 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 52 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110642.D
Acq On : 9 Nov 2018 22:03
Operator : JU/SJ
Sample : J5813-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

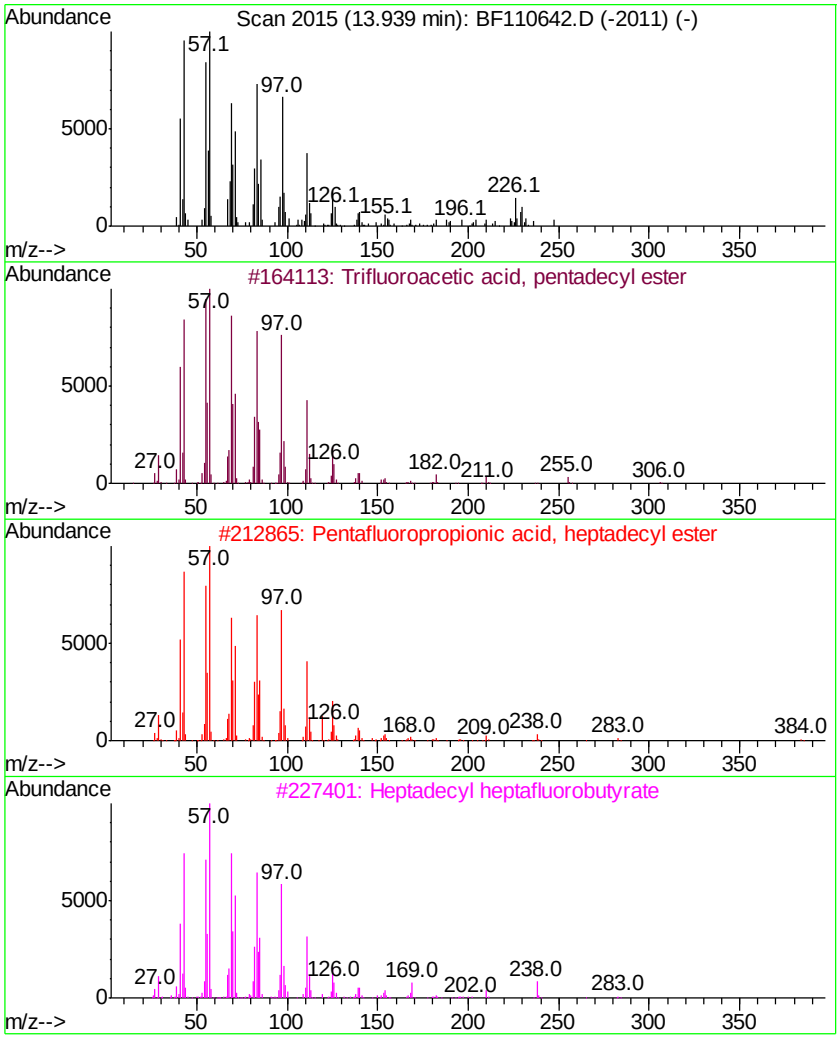
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

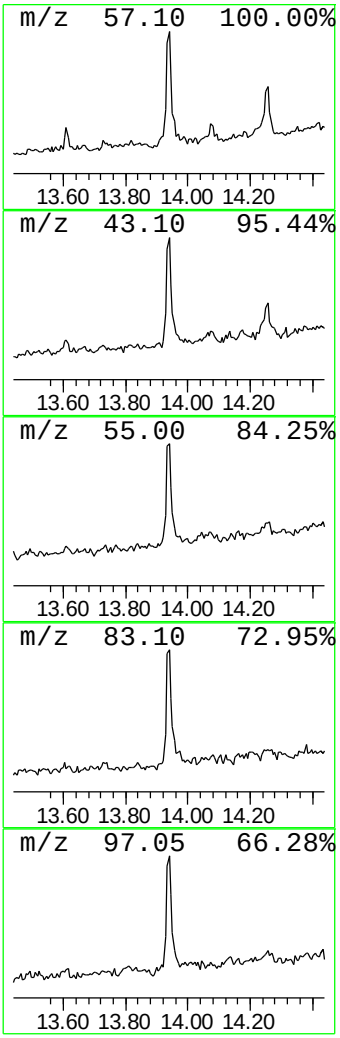
**********

Peak Number 6 Trifluoroacetic acid, penta... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.94 | 5.93 ng | 150233 | Chrysene-d12 | 14.13 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2 | 959010-23-2 | 93 |
| 2 | Pentafluoropropionic acid, hepta... | 402 | C20H35F5O2 | 959218-78-1 | 93 |
| 3 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 93 |
| 4 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 93 |
| 5 | Octadecyl trifluoroacetate | 366 | C20H37F3O2 | 079392-43-1 | 93 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110642.D
Acq On : 9 Nov 2018 22:03
Operator : JU/SJ
Sample : J5813-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

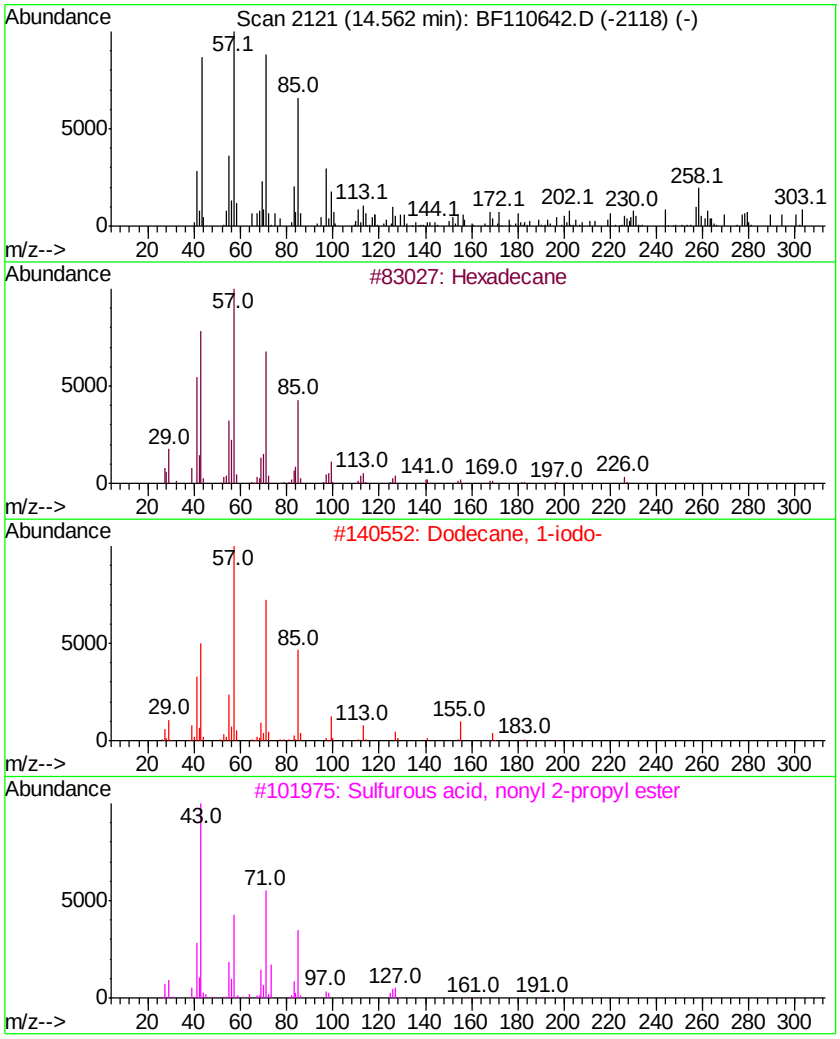
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

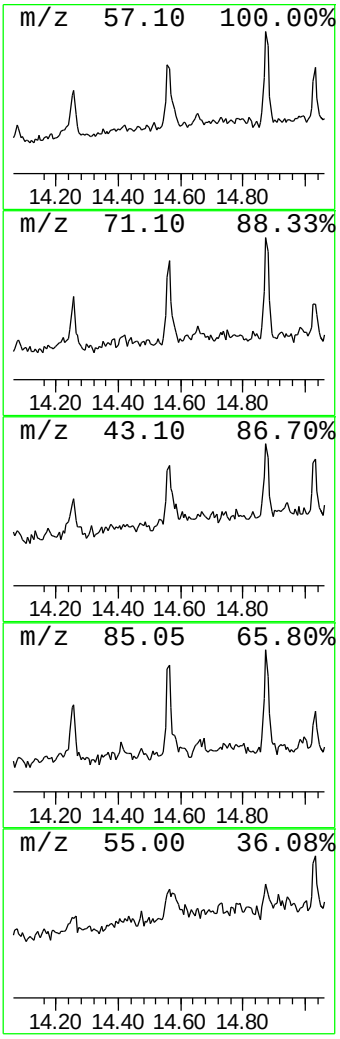
**********

Peak Number 7 Hexadecane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.56 | 2.75 ng | 69779 | Chrysene-d12 | 14.13 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane | 226 | C16H34 | 000544-76-3 | 58 |
| 2 | Dodecane, 1-iodo- | 296 | C12H25I | 004292-19-7 | 52 |
| 3 | Sulfurous acid, nonyl 2-propyl e... | 250 | C12H26O3S | 1000309-12-0 | 50 |
| 4 | Triacontane | 422 | C30H62 | 000638-68-6 | 50 |
| 5 | Dodecane, 4-methyl- | 184 | C13H28 | 006117-97-1 | 49 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110642.D
Acq On : 9 Nov 2018 22:03
Operator : JU/SJ
Sample : J5813-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

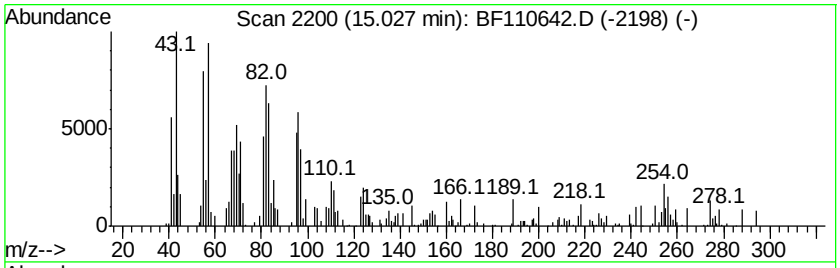
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

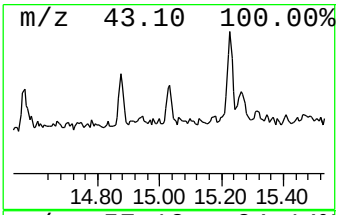
**********

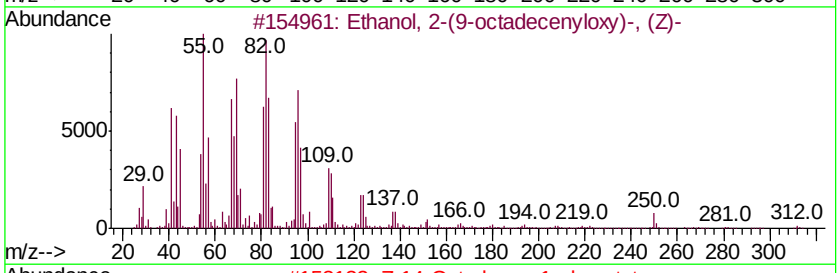
Peak Number 8 Ethanol, 2-(9-octadecenylox... Concentration Rank 6

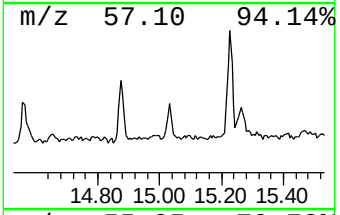
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.03 | 4.03 ng | 64901 | Perylene-d12 | 15.66 |

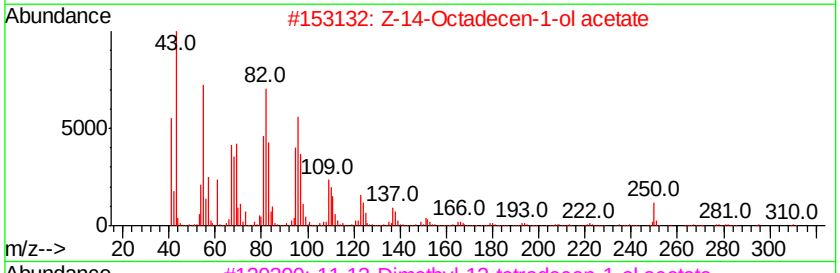
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2-(9-octadecenyloxy)-, ... | 312 | C20H40O2 | 005353-25-3 | 64 |
| 2 | Z-14-Octadecen-1-ol acetate | 310 | C20H38O2 | 1000131-07-6 | 64 |
| 3 | 11,13-Dimethyl-12-tetradecen-1-o... | 282 | C18H34O2 | 1000130-81-0 | 64 |
| 4 | Octadecanal | 268 | C18H36O | 000638-66-4 | 62 |
| 5 | 1,16-Hexadecanediol | 258 | C16H34O2 | 007735-42-4 | 60 |

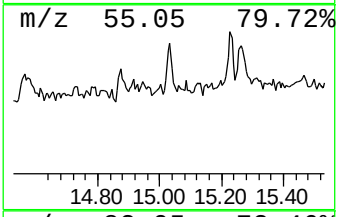


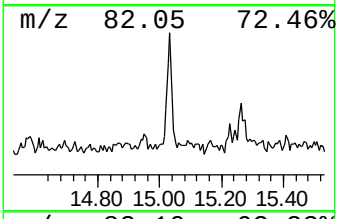



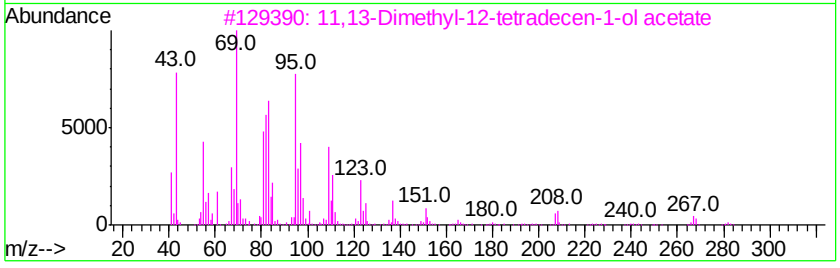



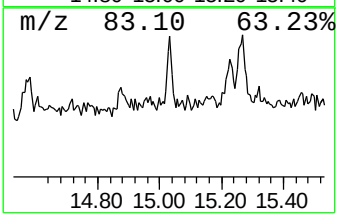



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110918\
Data File : BF110642.D
Acq On : 9 Nov 2018 22:03
Operator : JU/SJ
Sample : J5813-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

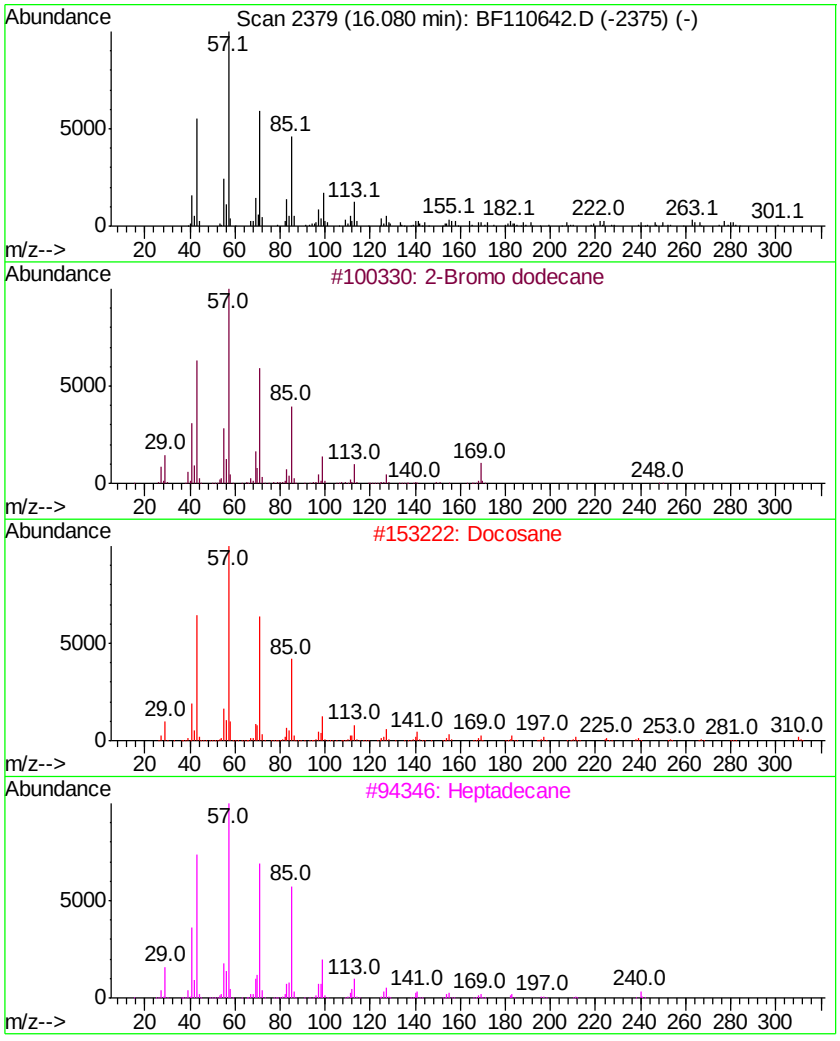
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

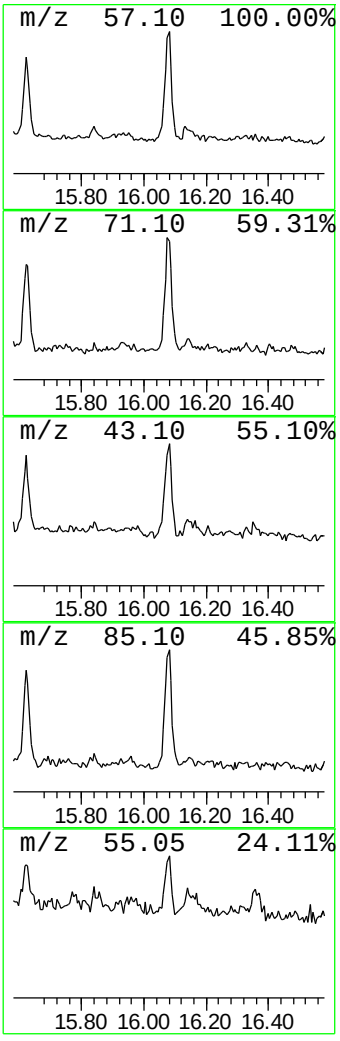
**********

Peak Number 9 2-Bromo dodecane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.08 | 8.32 ng | 133903 | Perylene-d12 | 15.66 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Bromo dodecane | 248 | C12H25Br | 013187-99-0 | 86 |
| 2 | Docosane | 310 | C22H46 | 000629-97-0 | 86 |
| 3 | Heptadecane | 240 | C17H36 | 000629-78-7 | 81 |
| 4 | Eicosane | 282 | C20H42 | 000112-95-8 | 80 |
| 5 | 6,6-Diethylhoctadecane | 310 | C22H46 | 1000360-41-8 | 80 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110918\
Data File : BF110642.D
Acq On : 9 Nov 2018 22:03
Operator : JU/SJ
Sample : J5813-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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 |
| Butane, 2-methoxy... | 2.25 | 14.1 | ng | 352487 | 1 | 6.95 | 498523 | 20.0 |
| 2-Pentanone, 4-hy... | 5.18 | 2.7 | ng | 67802 | 1 | 6.95 | 498523 | 20.0 |
| unknown6.72 | 6.72 | 72.8 | ng | 1815460 | 1 | 6.95 | 498523 | 20.0 |
| n-Hexadecanoic acid | 11.98 | 2.6 | ng | 76609 | 4 | 11.48 | 581039 | 20.0 |
| Trifluoroacetic a... | 13.94 | 5.9 | ng | 150233 | 5 | 14.13 | 506854 | 20.0 |
| Hexadecane | 14.56 | 2.8 | ng | 69779 | 5 | 14.13 | 506854 | 20.0 |
| Ethanol, 2-(9-oct... | 15.03 | 4.0 | ng | 64901 | 6 | 15.66 | 322057 | 20.0 |
| 2-Bromo dodecane | 16.08 | 8.3 | ng | 133903 | 6 | 15.66 | 322057 | 20.0 |