LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101518\
Data File : BF109898.D
Acq On : 15 Oct 2018 23:56
Operator : JU/SJ
Sample : J5198-19 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CL-02-101218-E

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-BF101518.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 | 2.281 | 29 | 33 | 46 | rVB | 375010 | 526115 | 27.06% | 2.149% |
| 2 | 5.198 | 526 | 529 | 535 | rVB | 80976 | 81669 | 4.20% | 0.334% |
| 3 | 5.586 | 591 | 595 | 599 | rBV | 2095645 | 1944038 | 100.00% | 7.942% |
| 4 | 6.586 | 761 | 765 | 769 | rBV | 2270669 | 1844793 | 94.89% | 7.536% |
| 5 | 6.739 | 788 | 791 | 795 | rBV | 2048106 | 1884163 | 96.92% | 7.697% |
| 6 | 6.980 | 828 | 832 | 835 | rVB | 1406580 | 1170225 | 60.20% | 4.781% |
| 7 | 7.133 | 854 | 858 | 861 | rBV | 1856073 | 1457747 | 74.99% | 5.955% |
| 8 | 7.533 | 922 | 926 | 929 | rBV | 1312819 | 1016762 | 52.30% | 4.154% |
| 9 | 8.263 | 1046 | 1050 | 1053 | rBV | 1568237 | 1305270 | 67.14% | 5.332% |
| 10 | 9.333 | 1228 | 1232 | 1235 | rBV | 2136755 | 1592061 | 81.89% | 6.504% |
| 11 | 9.410 | 1241 | 1245 | 1252 | rBV5 | 40125 | 57764 | 2.97% | 0.236% |
| 12 | 9.721 | 1295 | 1298 | 1302 | rBV | 247195 | 205068 | 10.55% | 0.838% |
| 13 | 9.880 | 1322 | 1325 | 1328 | rBV2 | 46965 | 43524 | 2.24% | 0.178% |
| 14 | 9.927 | 1331 | 1333 | 1336 | rVB2 | 52948 | 50182 | 2.58% | 0.205% |
| 15 | 10.021 | 1345 | 1349 | 1352 | rVB | 1359532 | 1263594 | 65.00% | 5.162% |
| 16 | 10.051 | 1352 | 1354 | 1360 | rVB3 | 28064 | 30541 | 1.57% | 0.125% |
| 17 | 10.427 | 1414 | 1418 | 1422 | rVB4 | 33052 | 41380 | 2.13% | 0.169% |
| 18 | 10.568 | 1438 | 1442 | 1447 | rVB2 | 29819 | 30811 | 1.58% | 0.126% |
| 19 | 10.804 | 1479 | 1482 | 1487 | rBV | 1206817 | 987277 | 50.78% | 4.033% |
| 20 | 10.921 | 1498 | 1502 | 1506 | rBV2 | 45160 | 56576 | 2.91% | 0.231% |
| 21 | 11.386 | 1578 | 1581 | 1583 | rBV | 22922 | 25098 | 1.29% | 0.103% |
| 22 | 11.510 | 1598 | 1602 | 1604 | rBV | 1779984 | 1432651 | 73.69% | 5.853% |
| 23 | 11.533 | 1604 | 1606 | 1612 | rVV | 180445 | 157281 | 8.09% | 0.643% |
| 24 | 11.580 | 1612 | 1614 | 1617 | rVB | 57053 | 49285 | 2.54% | 0.201% |
| 25 | 11.739 | 1639 | 1641 | 1646 | rBV6 | 18918 | 24412 | 1.26% | 0.100% |
| 26 | 12.015 | 1684 | 1688 | 1690 | rBV3 | 162352 | 170150 | 8.75% | 0.695% |
| 27 | 12.121 | 1703 | 1706 | 1709 | rBV | 83067 | 89928 | 4.63% | 0.367% |
| 28 | 12.304 | 1734 | 1737 | 1739 | rBV2 | 32896 | 31925 | 1.64% | 0.130% |
| 29 | 12.562 | 1778 | 1781 | 1783 | rBV | 47297 | 47125 | 2.42% | 0.193% |
| 30 | 12.586 | 1783 | 1785 | 1789 | rVV4 | 30048 | 44037 | 2.27% | 0.180% |
| 31 | 12.721 | 1805 | 1808 | 1811 | rBV | 432507 | 368460 | 18.95% | 1.505% |
| 32 | 12.804 | 1820 | 1822 | 1823 | rBV2 | 38697 | 31340 | 1.61% | 0.128% |
| 33 | 12.874 | 1832 | 1834 | 1837 | rBV2 | 41726 | 40236 | 2.07% | 0.164% |
| 34 | 12.957 | 1842 | 1848 | 1854 | rBV | 507393 | 566957 | 29.16% | 2.316% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101518\
Data File : BF109898.D
Acq On : 15 Oct 2018 23:56
Operator : JU/SJ
Sample : J5198-19 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CL-02-101218-E

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-BF101518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 13.092 | 1868 | 1871 | 1874 | rBV | 2237637 | 1769596 | 91.03% | 7.229% |
| 36 | 13.280 | 1901 | 1903 | 1906 | rVB2 | 122919 | 100537 | 5.17% | 0.411% |
| 37 | 13.345 | 1912 | 1914 | 1916 | rVB | 64569 | 47482 | 2.44% | 0.194% |
| 38 | 13.974 | 2018 | 2021 | 2028 | rBV | 449915 | 450003 | 23.15% | 1.838% |
| 39 | 14.151 | 2047 | 2051 | 2054 | rBV | 1669653 | 1679153 | 86.37% | 6.860% |
| 40 | 14.609 | 2127 | 2129 | 2136 | rVB2 | 279993 | 302110 | 15.54% | 1.234% |
| 41 | 15.286 | 2241 | 2244 | 2247 | rBV | 306243 | 359238 | 18.48% | 1.468% |
| 42 | 15.680 | 2307 | 2311 | 2318 | rVB | 779096 | 1102001 | 56.69% | 4.502% |

Sum of corrected areas: 24478565

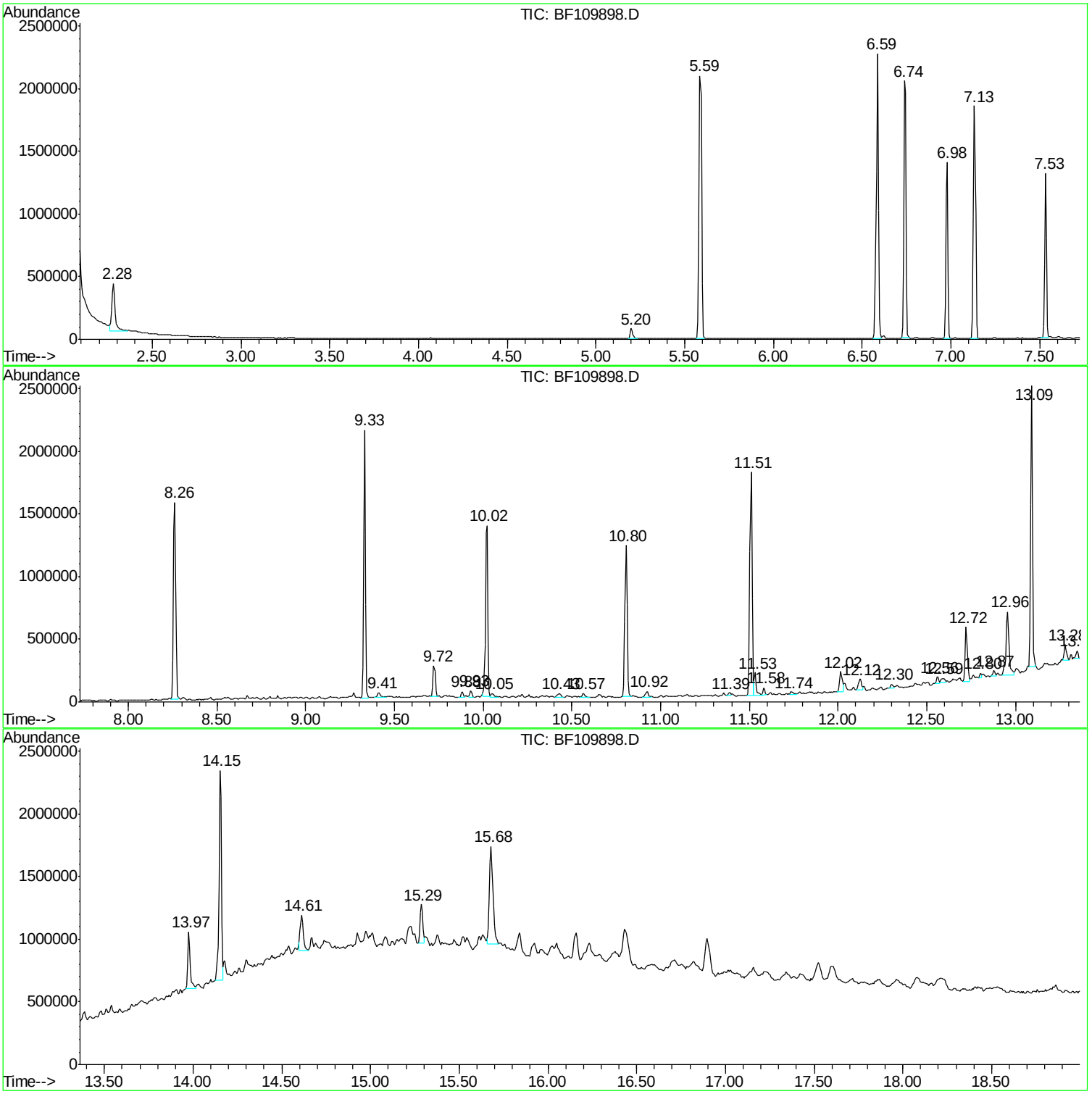
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101518\
Data File : BF109898.D
Acq On : 15 Oct 2018 23:56
Operator : JU/SJ
Sample : J5198-19 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CL-02-101218-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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\BF101518\
Data File : BF109898.D
Acq On : 15 Oct 2018 23:56
Operator : JU/SJ
Sample : J5198-19 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CL-02-101218-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

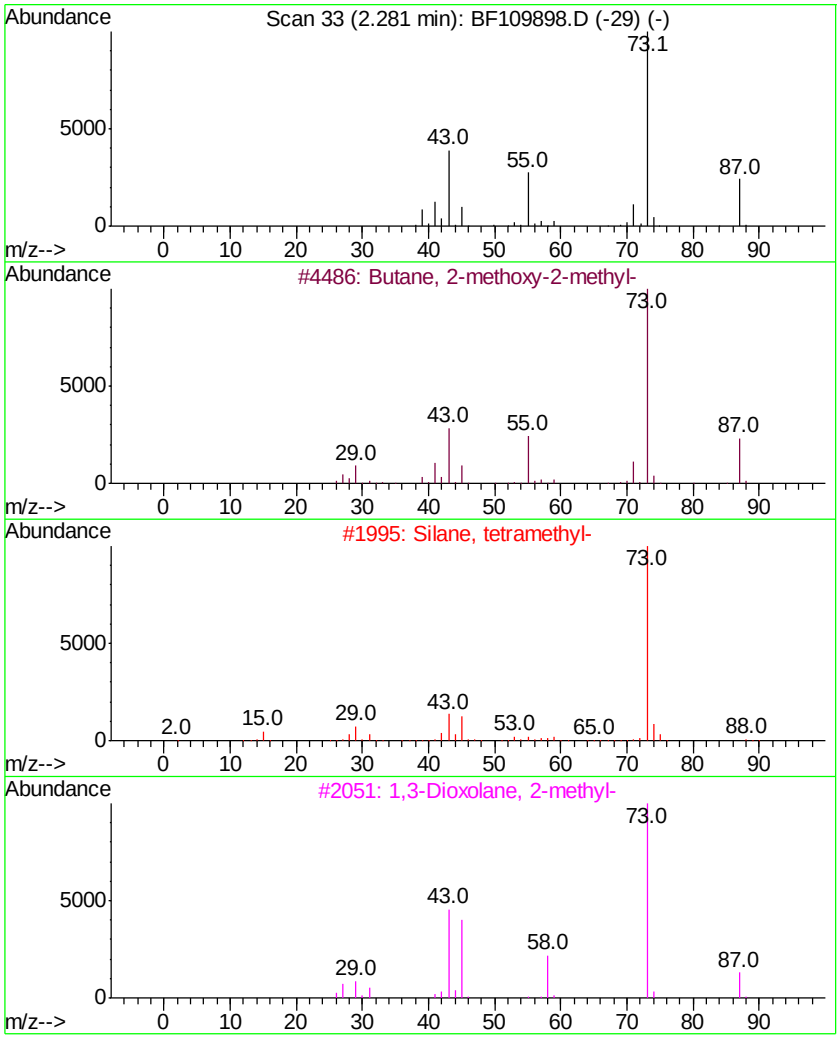
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

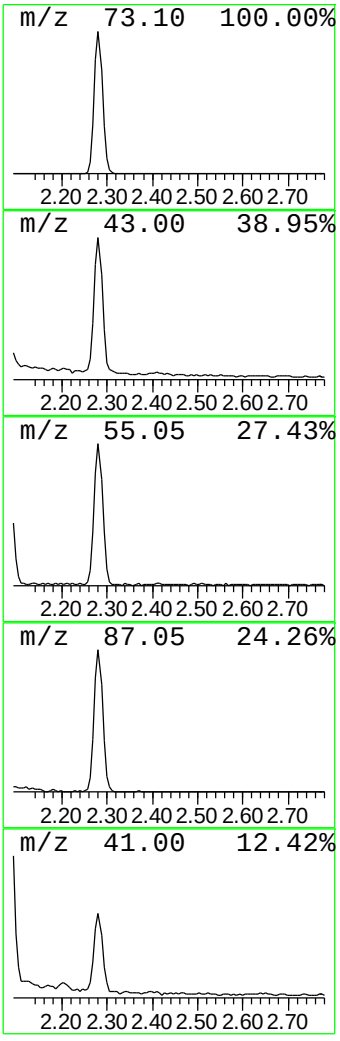
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.28 | 8.99 ng | 526115 | 1,4-Dichlorobenzene-d4 | 6.98 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 83 |
| 2 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 27 |
| 3 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 25 |
| 4 | Acetamide, N-ethyl- | 87 | C4H9NO | 000625-50-3 | 16 |
| 5 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 12 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101518\
Data File : BF109898.D
Acq On : 15 Oct 2018 23:56
Operator : JU/SJ
Sample : J5198-19 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CL-02-101218-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

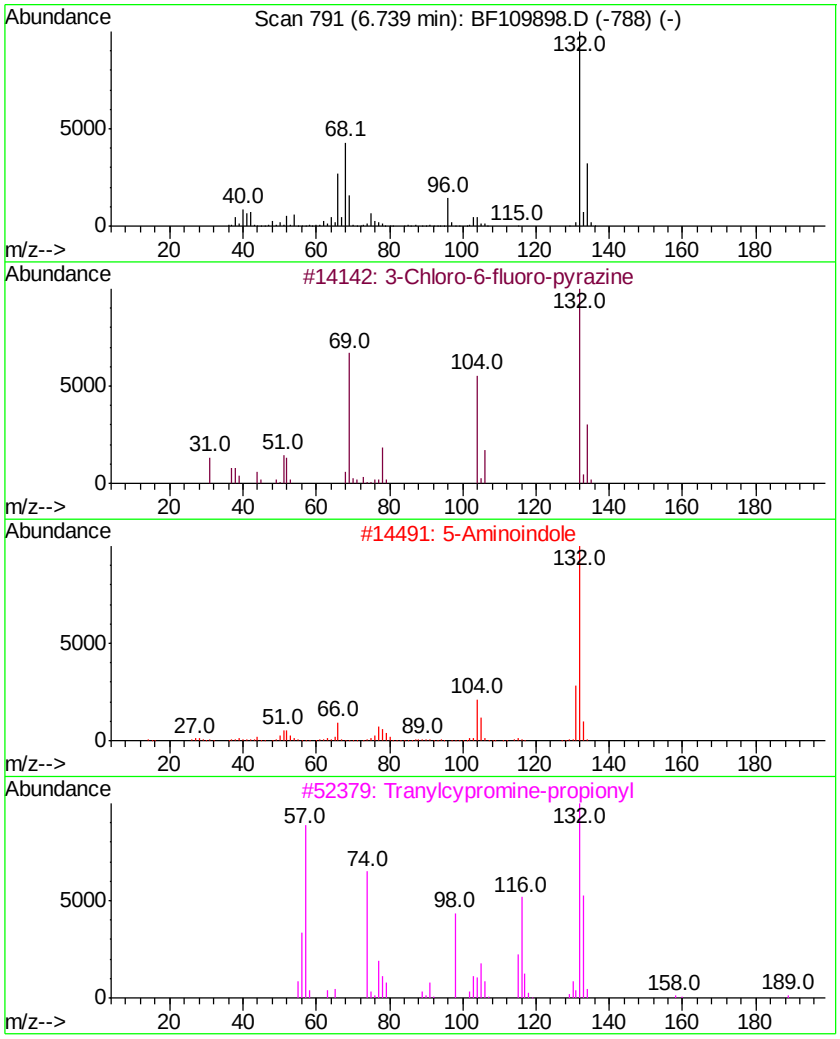
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

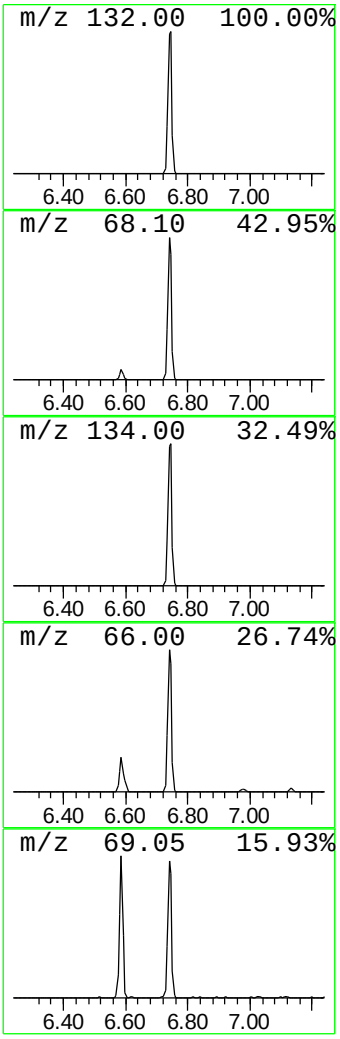
**********

Peak Number 2 unknown6.74 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.74 | 32.20 ng | 1884160 | 1,4-Dichlorobenzene-d4 | 6.98 |

| 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 | 4-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-60-2 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101518\
Data File : BF109898.D
Acq On : 15 Oct 2018 23:56
Operator : JU/SJ
Sample : J5198-19 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CL-02-101218-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

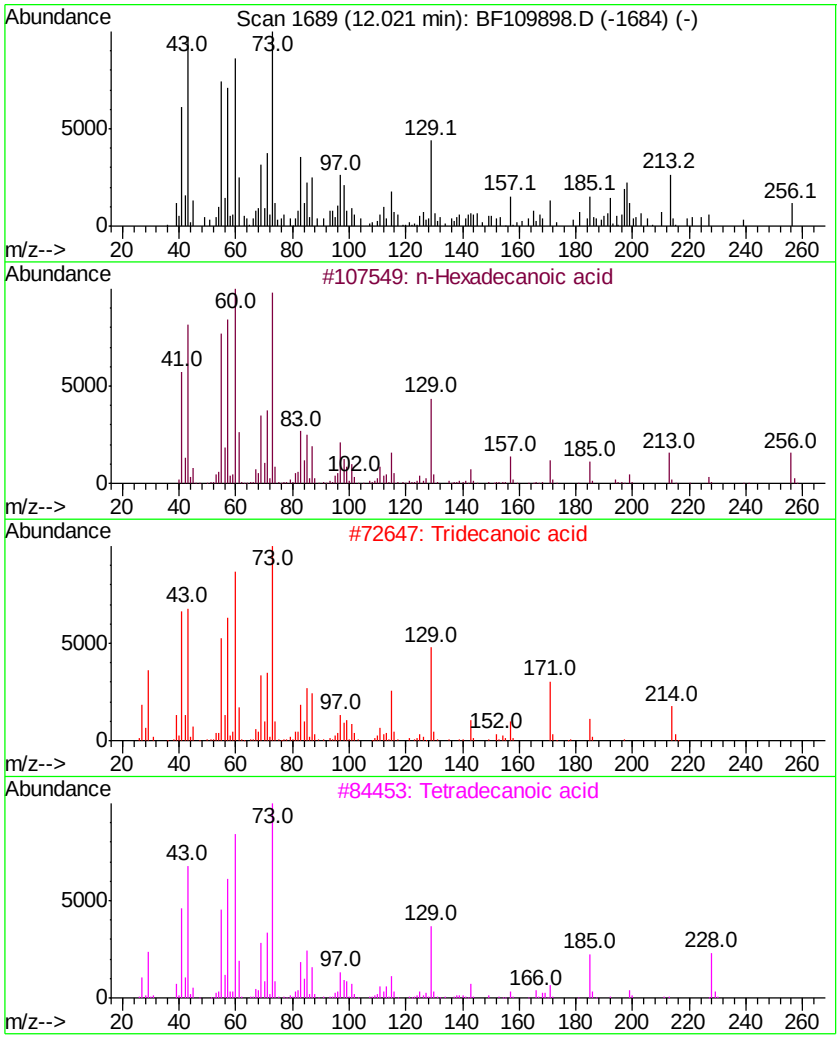
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

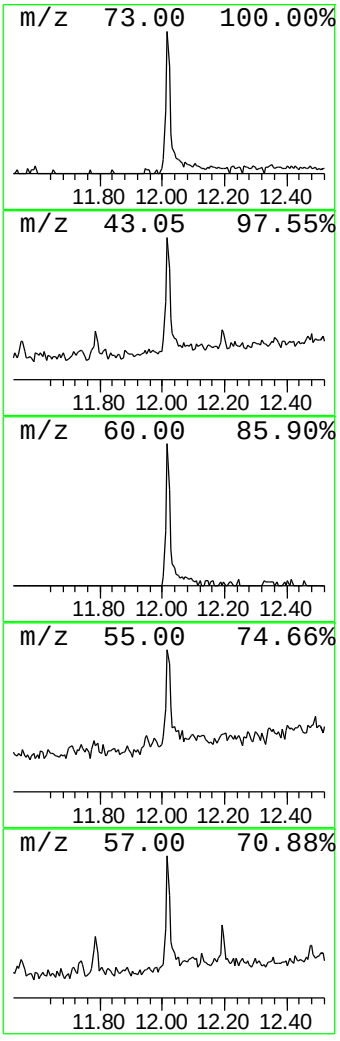
**********

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.02 | 2.38 ng | 170150 | Phenanthrene-d10 | 11.51 |

| 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 | 62 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 58 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 53 |
| 5 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 49 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101518\
Data File : BF109898.D
Acq On : 15 Oct 2018 23:56
Operator : JU/SJ
Sample : J5198-19 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CL-02-101218-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

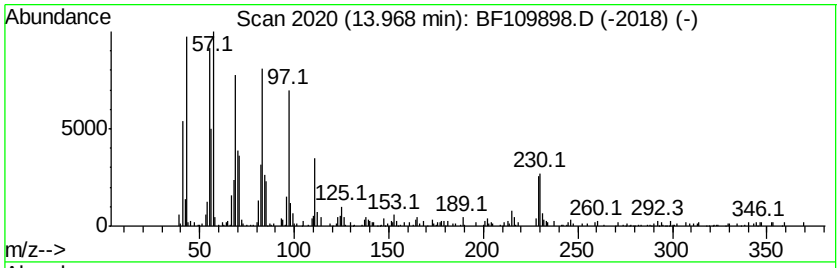
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

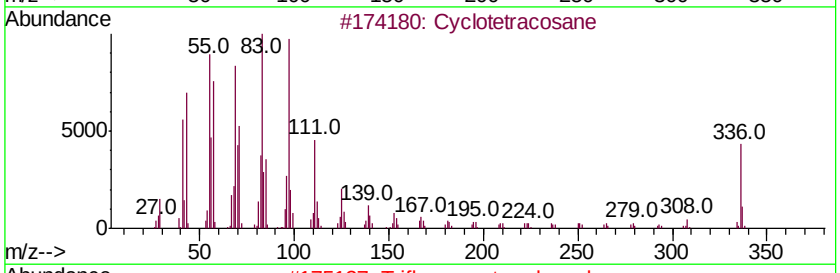
**********

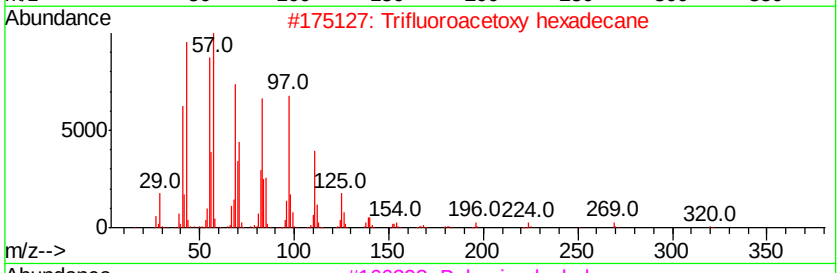
Peak Number 5 Cyclotetracosane Concentration Rank 5

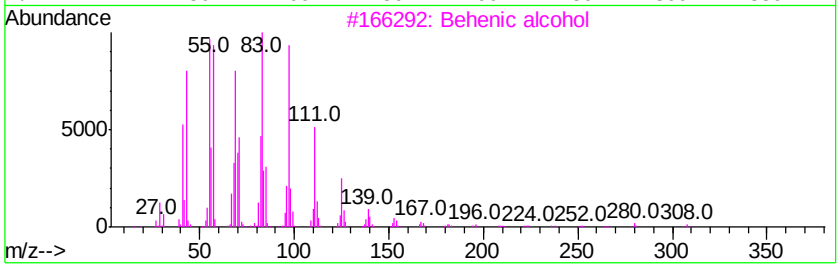
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.97 | 5.36 ng | 450003 | Chrysene-d12 | 14.15 |

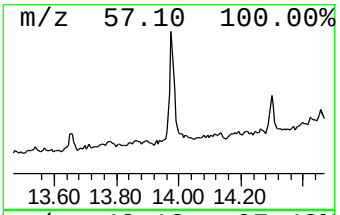
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclotetracosane | 336 | C24H48 | 000297-03-0 | 95 |
| 2 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 94 |
| 3 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 93 |
| 4 | 1-Heneicosyl formate | 340 | C22H44O2 | 077899-03-7 | 91 |
| 5 | Heptafluorobutyric acid, hexadec... | 438 | C20H33F7O2 | 006385-15-5 | 91 |

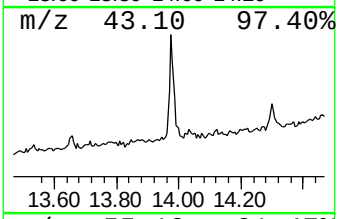


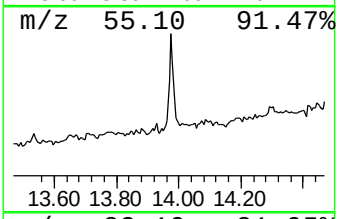



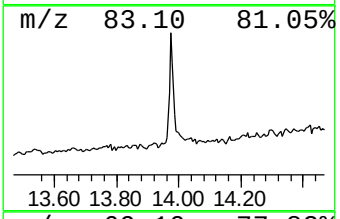



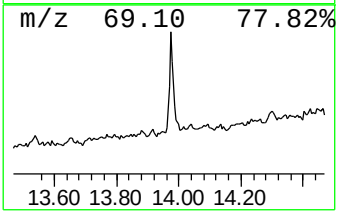



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101518\
Data File : BF109898.D
Acq On : 15 Oct 2018 23:56
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Sample : J5198-19 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CL-02-101218-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

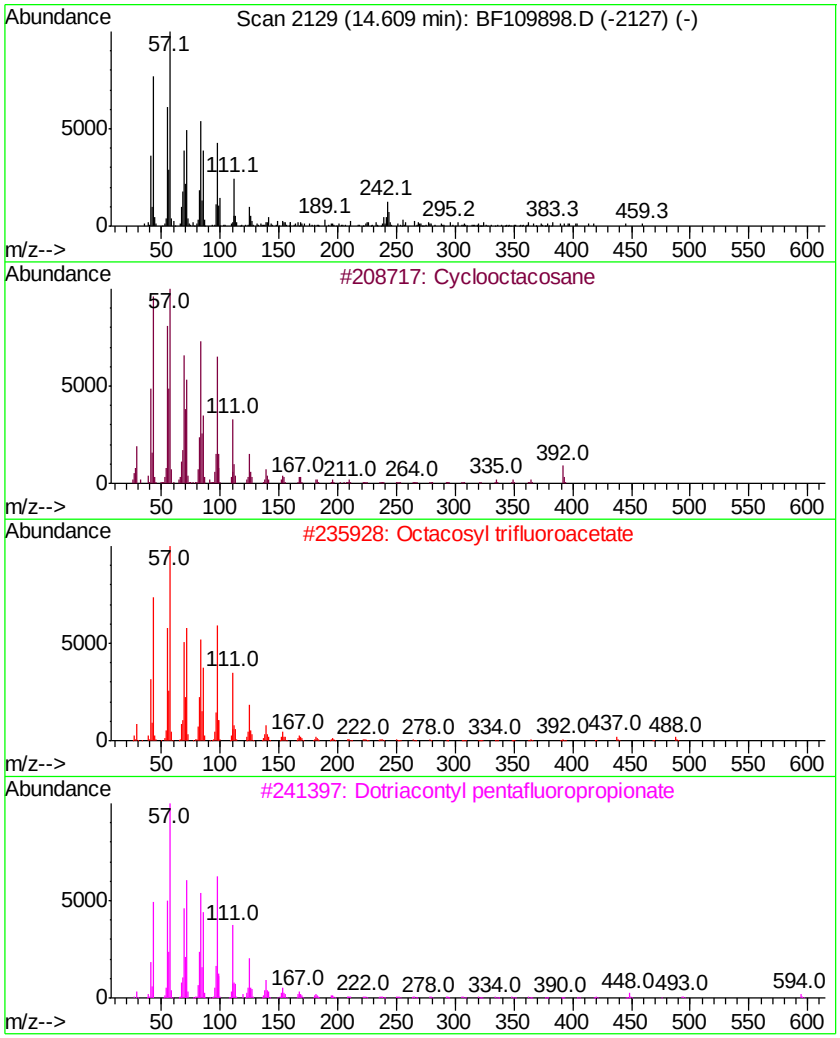
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

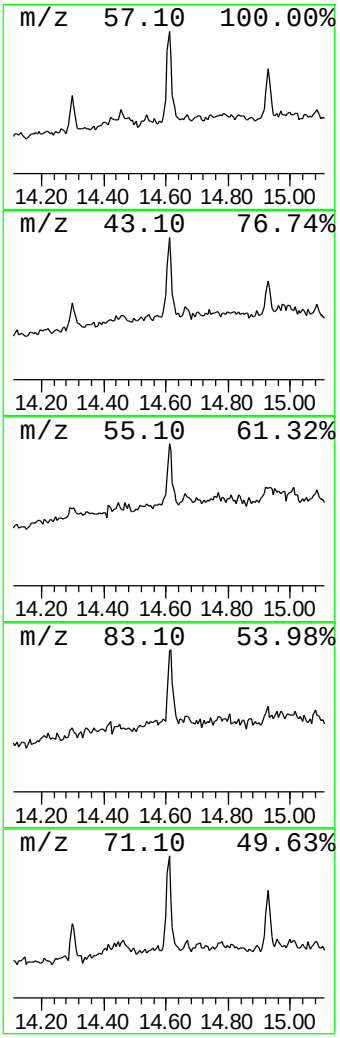
**********

Peak Number 6 Cyclooctacosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.61 | 3.60 ng | 302110 | Chrysene-d12 | 14.15 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclooctacosane | 392 | C28H56 | 000297-24-5 | 90 |
| 2 | Octacosyl trifluoroacetate | 506 | C30H57F3O2 | 1000351-74-9 | 90 |
| 3 | Dotriacontyl pentafluoropropionate | 612 | C35H65F5O2 | 1000351-81-4 | 90 |
| 4 | Octacosyl heptafluorobutyrate | 606 | C32H57F7O2 | 1000351-83-6 | 90 |
| 5 | Hexacosyl heptafluorobutyrate | 578 | C30H53F7O2 | 1000351-83-3 | 87 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101518\
Data File : BF109898.D
Acq On : 15 Oct 2018 23:56
Operator : JU/SJ
Sample : J5198-19 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CL-02-101218-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

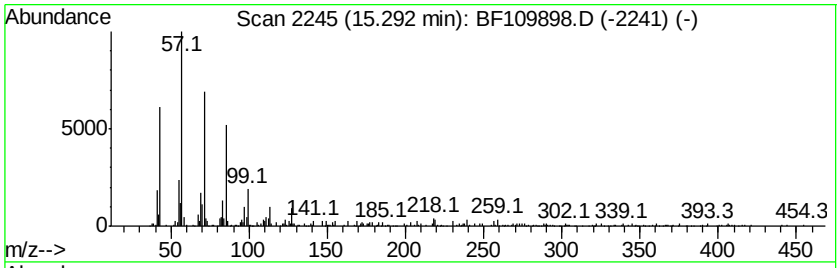
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

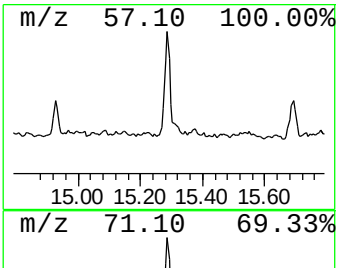
**********

Peak Number 7 Tetracosane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.29 | 6.52 ng | 359238 | Perylene-d12 | 15.68 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetracosane | 338 | C24H50 | 000646-31-1 | 93 |
| 2 | Hexadecane | 226 | C16H34 | 000544-76-3 | 91 |
| 3 | Hexacosane | 366 | C26H54 | 000630-01-3 | 87 |
| 4 | Docosane | 310 | C22H46 | 000629-97-0 | 87 |
| 5 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 86 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101518\
Data File : BF109898.D
Acq On : 15 Oct 2018 23:56
Operator : JU/SJ
Sample : J5198-19 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CL-02-101218-E

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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... | 2.28 | 9.0 | ng | 526115 | 1 | 6.98 | 1170230 | 20.0 |
| unknown6.74 | 6.74 | 32.2 | ng | 1884160 | 1 | 6.98 | 1170230 | 20.0 |
| n-Hexadecanoic acid | 12.02 | 2.4 | ng | 170150 | 4 | 11.51 | 1432650 | 20.0 |
| Cyclotetracosane | 13.97 | 5.4 | ng | 450003 | 5 | 14.15 | 1679150 | 20.0 |
| Cyclooctacosane | 14.61 | 3.6 | ng | 302110 | 5 | 14.15 | 1679150 | 20.0 |
| Tetracosane | 15.29 | 6.5 | ng | 359238 | 6 | 15.68 | 1102000 | 20.0 |