LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112019\
Data File : BF117896.D
Acq On : 20 Nov 2019 16:39
Operator : JU
Sample : K5904-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 14-(2-4)

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-BF111319.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 | 2.199 | 13 | 19 | 32 | rVB | 538802 | 695158 | 21.86% | 2.356% |
| 2 | 4.516 | 408 | 413 | 420 | rBV | 697248 | 749841 | 23.58% | 2.541% |
| 3 | 5.140 | 510 | 519 | 522 | rBV | 1973095 | 2780537 | 87.45% | 9.424% |
| 4 | 5.528 | 581 | 585 | 591 | rBV | 646883 | 609543 | 19.17% | 2.066% |
| 5 | 6.534 | 752 | 756 | 768 | rBV | 2284298 | 2372823 | 74.63% | 8.042% |
| 6 | 6.681 | 777 | 781 | 784 | rBV | 1915851 | 1540578 | 48.45% | 5.221% |
| 7 | 6.734 | 788 | 790 | 796 | rVB | 52343 | 55625 | 1.75% | 0.189% |
| 8 | 6.916 | 817 | 821 | 824 | rBV | 1135197 | 866163 | 27.24% | 2.936% |
| 9 | 7.075 | 844 | 848 | 851 | rBV | 2622318 | 2203278 | 69.30% | 7.468% |
| 10 | 7.475 | 912 | 916 | 919 | rBV | 1963951 | 1756588 | 55.25% | 5.954% |
| 11 | 8.204 | 1036 | 1040 | 1043 | rBV | 1340184 | 1134320 | 35.68% | 3.845% |
| 12 | 9.280 | 1219 | 1223 | 1226 | rBV | 3964310 | 3179453 | 100.00% | 10.776% |
| 13 | 9.357 | 1233 | 1236 | 1239 | rBV | 38077 | 39112 | 1.23% | 0.133% |
| 14 | 9.622 | 1274 | 1281 | 1283 | rBV | 42378 | 48093 | 1.51% | 0.163% |
| 15 | 9.675 | 1287 | 1290 | 1294 | rVV | 323465 | 281047 | 8.84% | 0.953% |
| 16 | 9.892 | 1320 | 1327 | 1330 | rBV | 54149 | 56877 | 1.79% | 0.193% |
| 17 | 9.969 | 1336 | 1340 | 1343 | rBV | 1486701 | 1365981 | 42.96% | 4.630% |
| 18 | 9.998 | 1343 | 1345 | 1348 | rVB | 64442 | 49688 | 1.56% | 0.168% |
| 19 | 10.169 | 1369 | 1374 | 1378 | rVB | 47595 | 53141 | 1.67% | 0.180% |
| 20 | 10.392 | 1410 | 1412 | 1415 | rVB | 78982 | 58485 | 1.84% | 0.198% |
| 21 | 10.516 | 1429 | 1433 | 1436 | rBV | 56225 | 57812 | 1.82% | 0.196% |
| 22 | 10.616 | 1446 | 1450 | 1455 | rVB3 | 30465 | 45099 | 1.42% | 0.153% |
| 23 | 10.751 | 1468 | 1473 | 1478 | rBV | 233053 | 232518 | 7.31% | 0.788% |
| 24 | 10.869 | 1486 | 1493 | 1494 | rBV2 | 99831 | 103258 | 3.25% | 0.350% |
| 25 | 11.316 | 1566 | 1569 | 1572 | rBV | 146126 | 123044 | 3.87% | 0.417% |
| 26 | 11.351 | 1572 | 1575 | 1578 | rVV2 | 56085 | 45345 | 1.43% | 0.154% |
| 27 | 11.457 | 1589 | 1593 | 1596 | rBV | 1503891 | 1448187 | 45.55% | 4.908% |
| 28 | 11.480 | 1596 | 1597 | 1601 | rVV | 460241 | 310951 | 9.78% | 1.054% |
| 29 | 11.533 | 1603 | 1606 | 1609 | rVB | 99503 | 92340 | 2.90% | 0.313% |
| 30 | 11.686 | 1626 | 1632 | 1638 | rBV | 53181 | 88205 | 2.77% | 0.299% |
| 31 | 11.745 | 1640 | 1642 | 1646 | rVB2 | 74354 | 67936 | 2.14% | 0.230% |
| 32 | 11.857 | 1659 | 1661 | 1667 | rVB3 | 29802 | 40401 | 1.27% | 0.137% |
| 33 | 11.963 | 1675 | 1679 | 1680 | rBV | 76825 | 76003 | 2.39% | 0.258% |
| 34 | 12.074 | 1695 | 1698 | 1700 | rBV2 | 97682 | 112565 | 3.54% | 0.382% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112019\
Data File : BF117896.D
Acq On : 20 Nov 2019 16:39
Operator : JU
Sample : K5904-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 14-(2-4)

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-BF111319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 12.098 | 1700 | 1702 | 1705 | rVB | 60645 | 49502 | 1.56% | 0.168% |
| 36 | 12.157 | 1709 | 1712 | 1716 | rVB | 95005 | 81997 | 2.58% | 0.278% |
| 37 | 12.510 | 1769 | 1772 | 1775 | rBV2 | 54266 | 58074 | 1.83% | 0.197% |
| 38 | 12.545 | 1775 | 1778 | 1785 | rVV3 | 99663 | 154075 | 4.85% | 0.522% |
| 39 | 12.598 | 1785 | 1787 | 1793 | rVV3 | 43044 | 72886 | 2.29% | 0.247% |
| 40 | 12.674 | 1797 | 1800 | 1803 | rVB | 393228 | 314337 | 9.89% | 1.065% |
| 41 | 12.904 | 1834 | 1839 | 1845 | rBV | 355950 | 419156 | 13.18% | 1.421% |
| 42 | 13.045 | 1859 | 1863 | 1867 | rBV | 2939170 | 2647563 | 83.27% | 8.973% |
| 43 | 13.127 | 1873 | 1877 | 1879 | rBV3 | 34718 | 46932 | 1.48% | 0.159% |
| 44 | 13.233 | 1893 | 1895 | 1897 | rVB | 55346 | 40636 | 1.28% | 0.138% |
| 45 | 13.945 | 2013 | 2016 | 2026 | rBV | 206125 | 317209 | 9.98% | 1.075% |
| 46 | 14.104 | 2037 | 2043 | 2046 | rBV2 | 1048342 | 1143912 | 35.98% | 3.877% |
| 47 | 14.133 | 2046 | 2048 | 2056 | rVB | 141405 | 141158 | 4.44% | 0.478% |
| 48 | 15.162 | 2220 | 2223 | 2227 | rBV | 124175 | 192285 | 6.05% | 0.652% |
| 49 | 15.545 | 2286 | 2288 | 2295 | rVB | 90290 | 105555 | 3.32% | 0.358% |
| 50 | 15.615 | 2295 | 2300 | 2304 | rBV | 751268 | 979599 | 30.81% | 3.320% |

Sum of corrected areas: 29504871

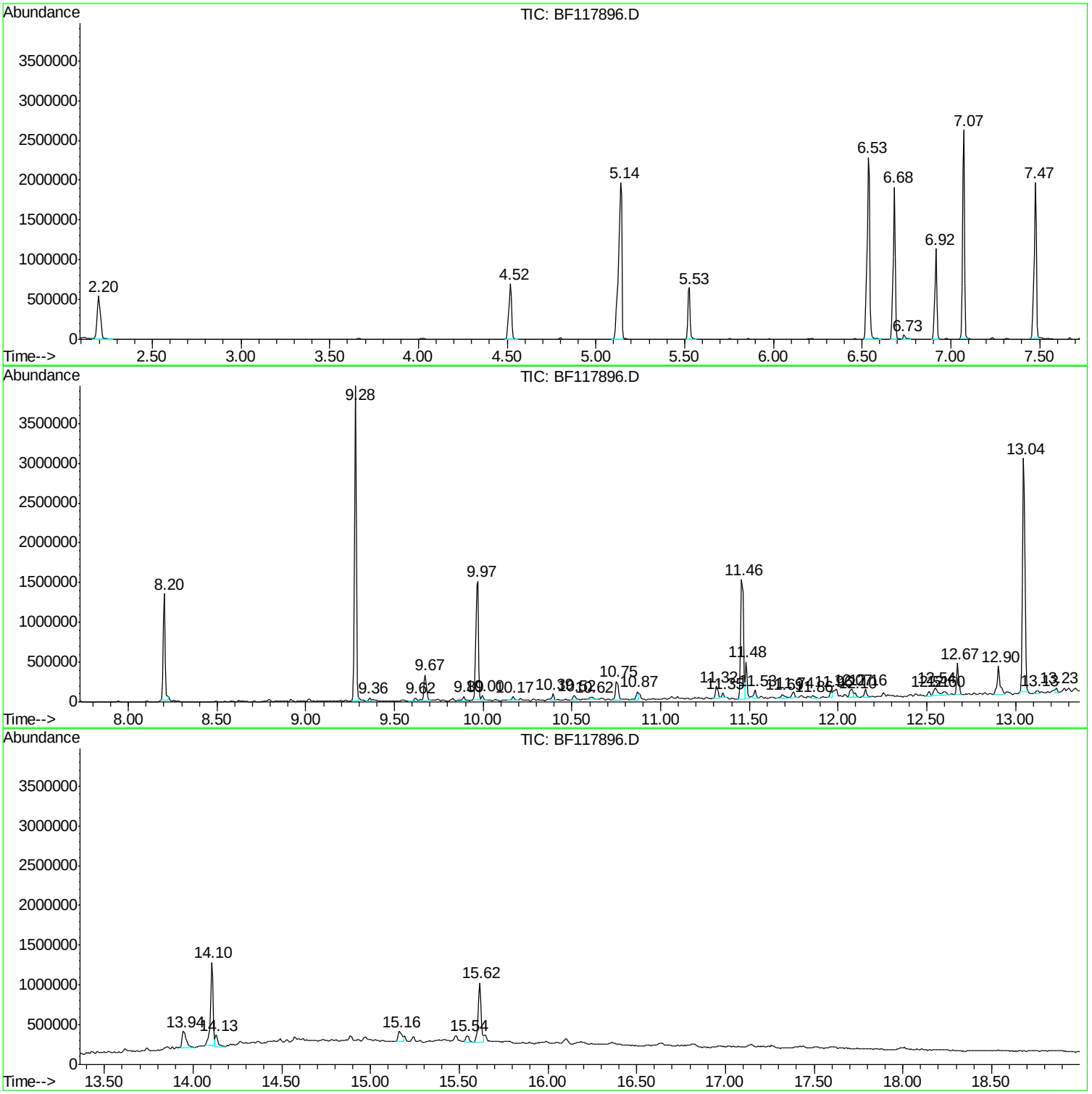
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112019\
Data File : BF117896.D
Acq On : 20 Nov 2019 16:39
Operator : JU
Sample : K5904-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
14-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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\BF112019\
Data File : BF117896.D
Acq On : 20 Nov 2019 16:39
Operator : JU
Sample : K5904-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 14-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

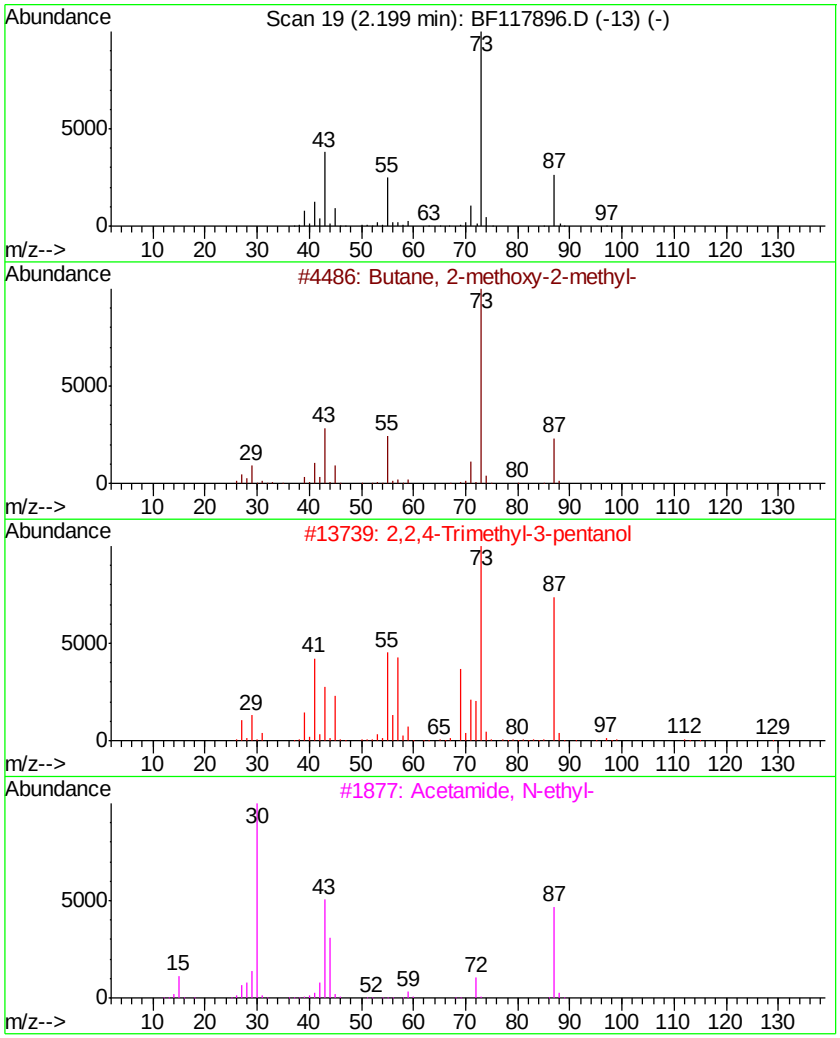
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

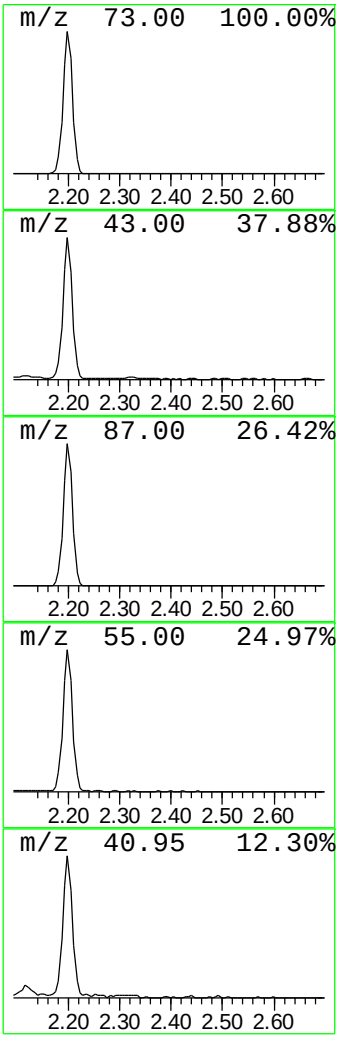
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.20 | 16.05 ng | 695158 | 1,4-Dichlorobenzene-d4 | 6.92 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 78 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 40 |
| 3 | Acetamide, N-ethyl- | 87 | C4H9NO | 000625-50-3 | 22 |
| 4 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 17 |
| 5 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 12 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112019\
Data File : BF117896.D
Acq On : 20 Nov 2019 16:39
Operator : JU
Sample : K5904-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 14-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

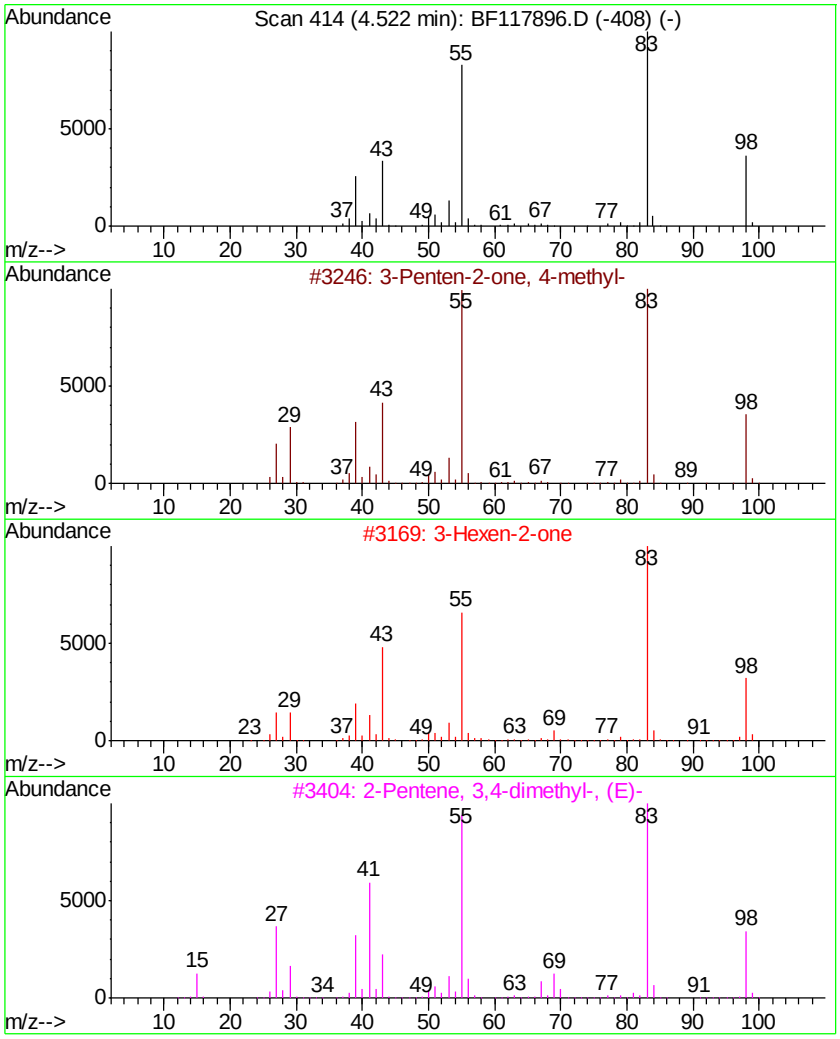
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

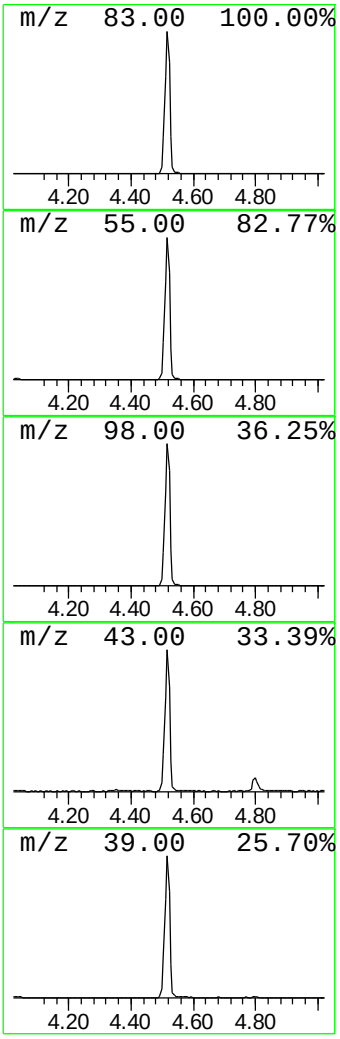
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.52 | 17.31 ng | 749841 | 1,4-Dichlorobenzene-d4 | 6.92 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Penten-2-one, 4-methyl- | 98 | C6H10O | 000141-79-7 | 95 |
| 2 | 3-Hexen-2-one | 98 | C6H10O | 000763-93-9 | 90 |
| 3 | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14 | 004914-92-5 | 90 |
| 4 | 2-Pentene, 4,4-dimethyl-, (Z)- | 98 | C7H14 | 000762-63-0 | 86 |
| 5 | 2-Pentene, 3,4-dimethyl-, (Z)- | 98 | C7H14 | 004914-91-4 | 86 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112019\
Data File : BF117896.D
Acq On : 20 Nov 2019 16:39
Operator : JU
Sample : K5904-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 14-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

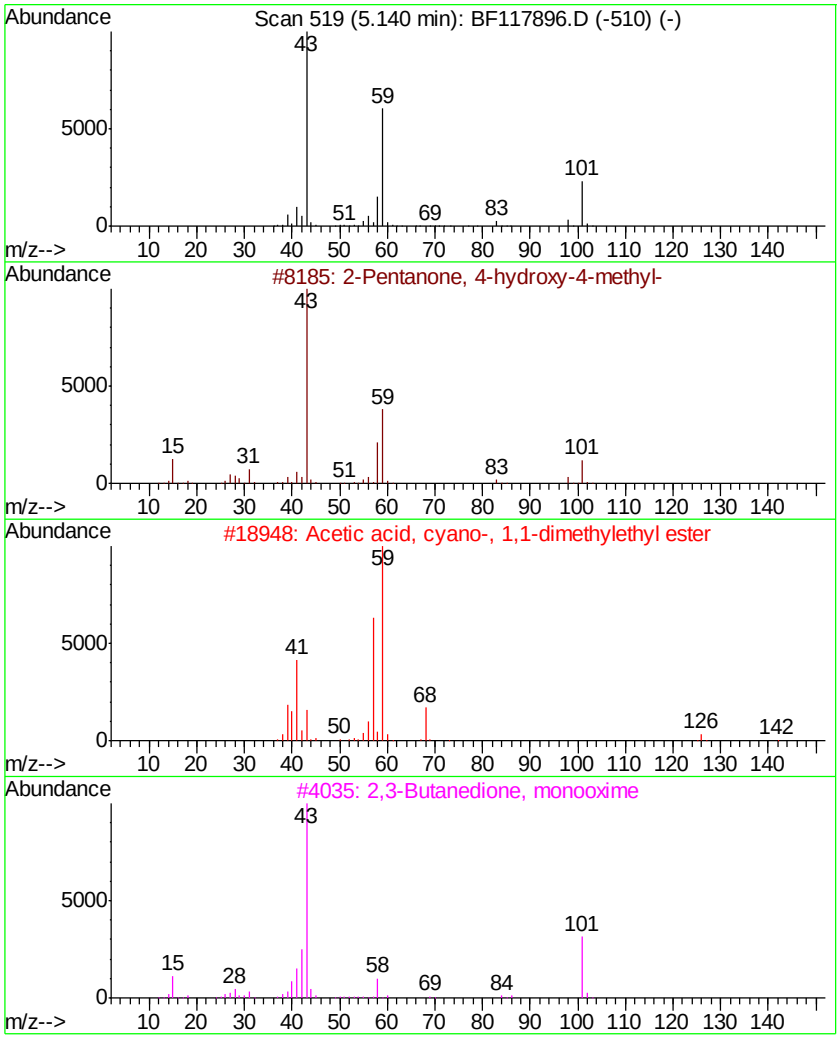
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

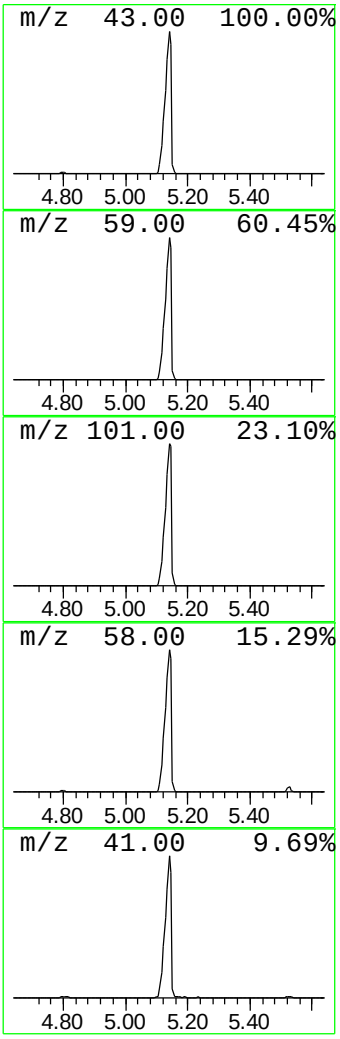
**********

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.14 | 64.20 ng | 2780540 | 1,4-Dichlorobenzene-d4 | 6.92 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 72 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 17 |
| 4 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |
| 5 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112019\
Data File : BF117896.D
Acq On : 20 Nov 2019 16:39
Operator : JU
Sample : K5904-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 14-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

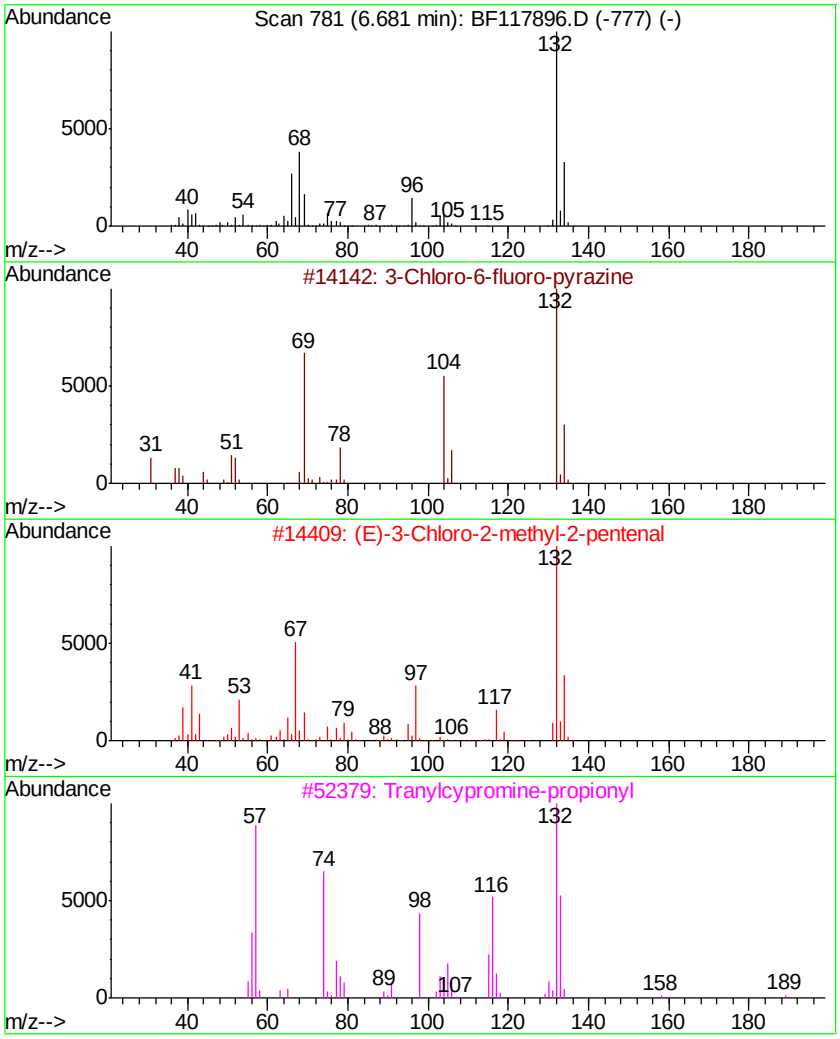
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

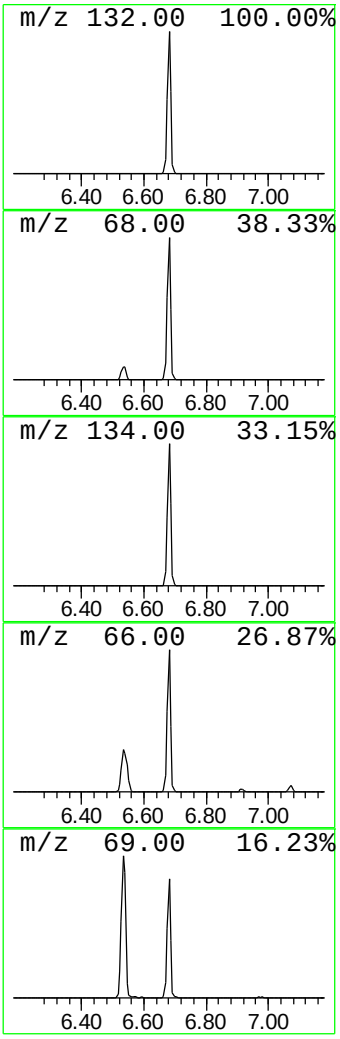
**********

Peak Number 4 unknown6.68 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.68 | 35.57 ng | 1540580 | 1,4-Dichlorobenzene-d4 | 6.92 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 12 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 4 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 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\BF112019\
Data File : BF117896.D
Acq On : 20 Nov 2019 16:39
Operator : JU
Sample : K5904-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 14-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

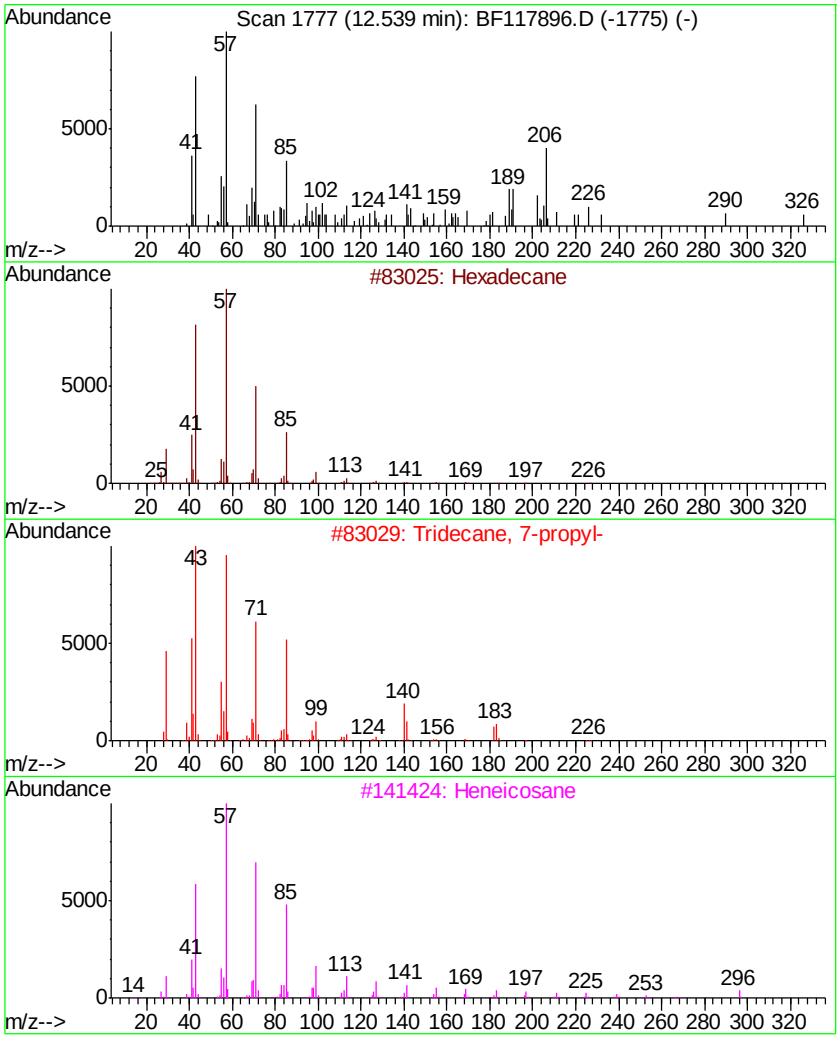
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

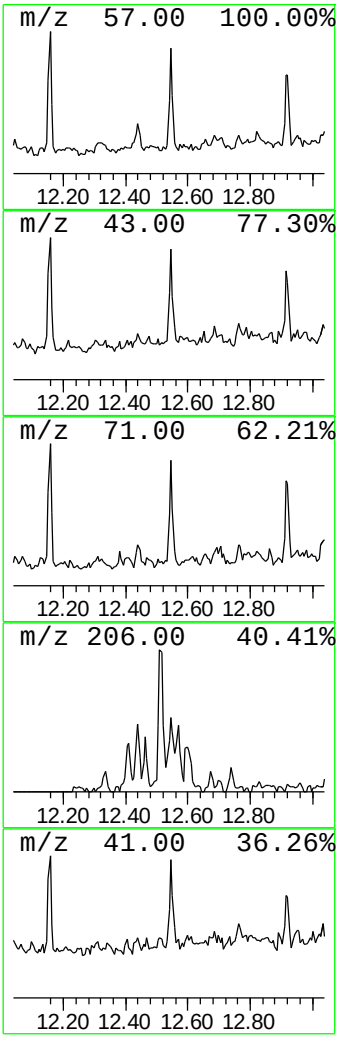
**********

Peak Number 6 Hexadecane Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.54 | 2.13 ng | 154075 | Phenanthrene-d10 | 11.46 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane | 226 | C16H34 | 000544-76-3 | 86 |
| 2 | Tridecane, 7-propyl- | 226 | C16H34 | 055045-09-5 | 43 |
| 3 | Heneicosane | 296 | C21H44 | 000629-94-7 | 41 |
| 4 | Tetracosane | 338 | C24H50 | 000646-31-1 | 41 |
| 5 | Octacosane | 394 | C28H58 | 000630-02-4 | 41 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112019\
Data File : BF117896.D
Acq On : 20 Nov 2019 16:39
Operator : JU
Sample : K5904-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 14-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

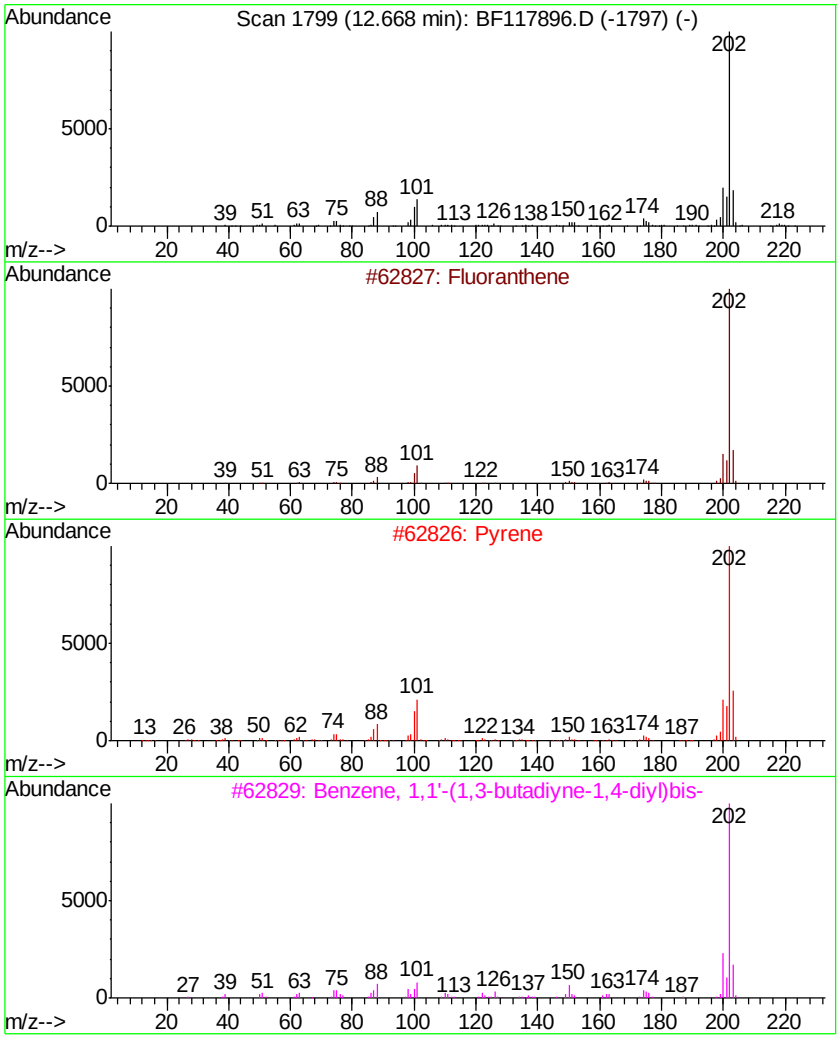
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

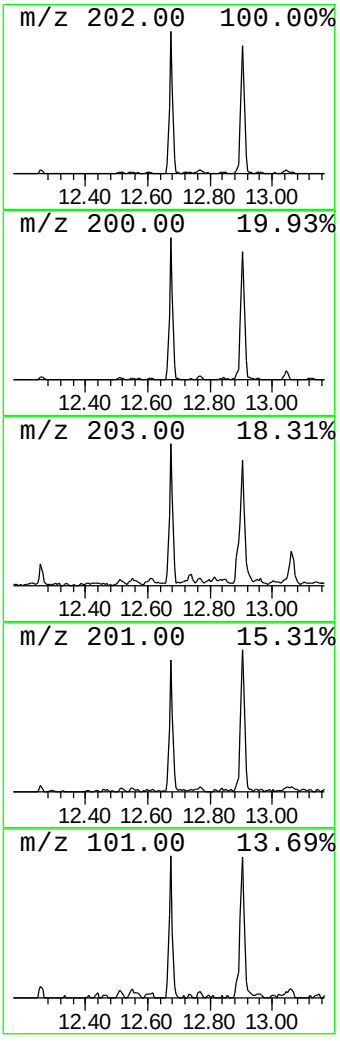
**********

Peak Number 7 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.67 | 4.34 ng | 314337 | Phenanthrene-d10 | 11.46 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Fluoranthene | 202 | C16H10 | 000206-44-0 | 96 |
| 2 | Pyrene | 202 | C16H10 | 000129-00-0 | 95 |
| 3 | Benzene, 1,1'-(1,3-butadiyne-1,4... | 202 | C16H10 | 000886-66-8 | 74 |
| 4 | 1,4-Pentadiyn-3-one, 1,5-diphenyl- | 230 | C17H10O | 015814-30-9 | 50 |
| 5 | 4,4'-Bis(tetrahydrothiopyran) | 202 | C10H18S2 | 116196-83-9 | 49 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112019\
Data File : BF117896.D
Acq On : 20 Nov 2019 16:39
Operator : JU
Sample : K5904-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 14-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

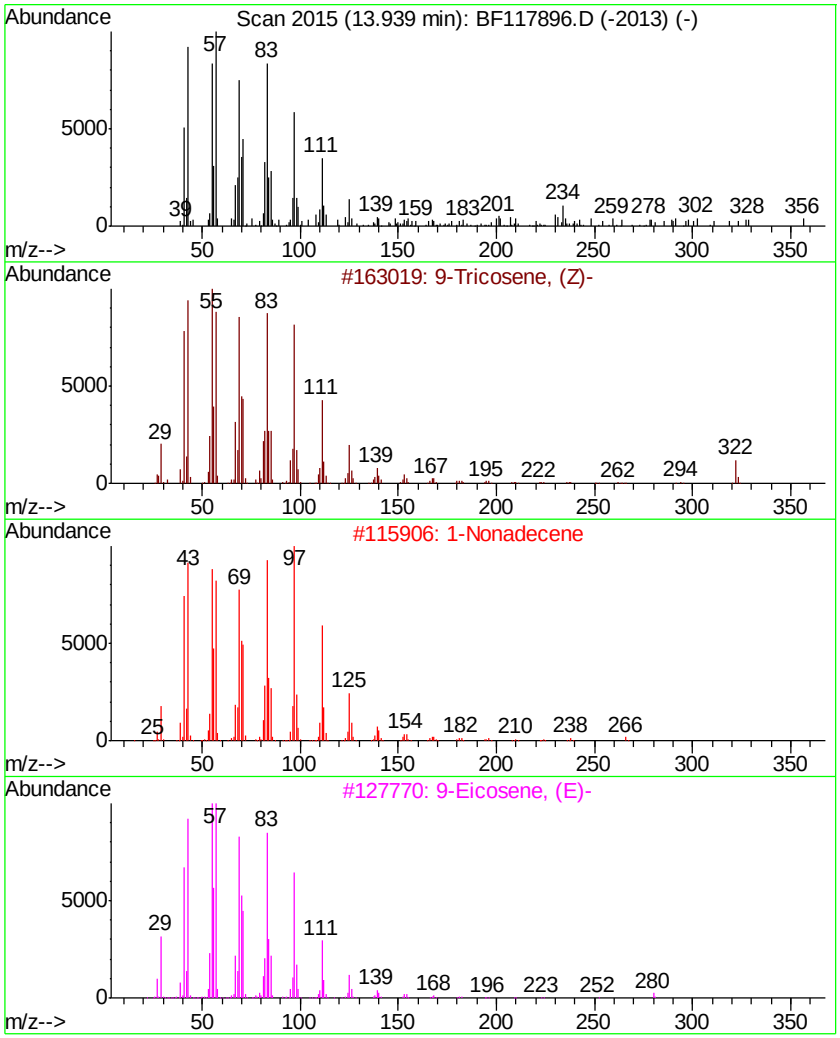
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

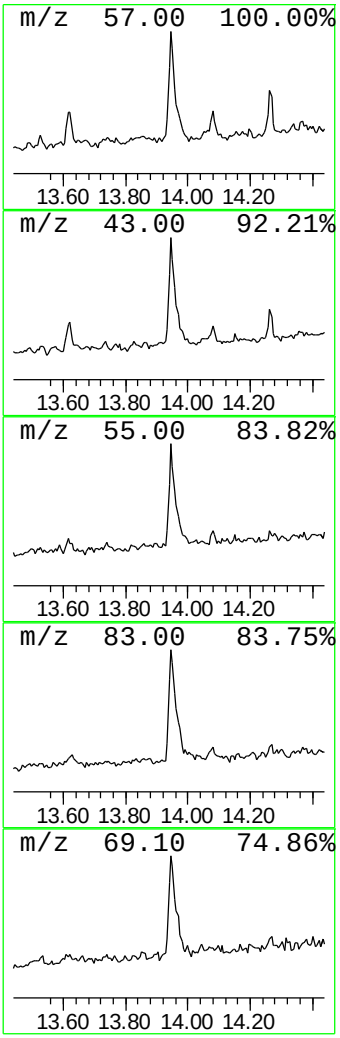
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.94 | 5.55 ng | 317209 | Chrysene-d12 | 14.10 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9-Tricosene, (Z)- | 322 | C23H46 | 027519-02-4 | 93 |
| 2 | 1-Nonadecene | 266 | C19H38 | 018435-45-5 | 92 |
| 3 | 9-Eicosene, (E)- | 280 | C20H40 | 074685-29-3 | 92 |
| 4 | 3-Eicosene, (E)- | 280 | C20H40 | 074685-33-9 | 92 |
| 5 | Heptafluorobutyric acid, hexadec... | 438 | C20H33F7O2 | 006385-15-5 | 91 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112019\
Data File : BF117896.D
Acq On : 20 Nov 2019 16:39
Operator : JU
Sample : K5904-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 14-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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... | 2.20 | 16.1 | ng | 695158 | 1 | 6.92 | 866163 | 20.0 |
| 3-Penten-2-one, 4... | 4.52 | 17.3 | ng | 749841 | 1 | 6.92 | 866163 | 20.0 |
| 2-Pentanone, 4-hy... | 5.14 | 64.2 | ng | 2780540 | 1 | 6.92 | 866163 | 20.0 |
| unknown6.68 | 6.68 | 35.6 | ng | 1540580 | 1 | 6.92 | 866163 | 20.0 |
| Hexadecane | 12.54 | 2.1 | ng | 154075 | 4 | 11.46 | 1448190 | 20.0 |
| Benzene, 1,1'-(1,... | 12.67 | 4.3 | ng | 314337 | 4 | 11.46 | 1448190 | 20.0 |
| 9-Tricosene, (Z)- | 13.94 | 5.5 | ng | 317209 | 5 | 14.10 | 1143910 | 20.0 |