LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112220.D
Acq On : 24 Jan 2019 20:29
Operator : JU/SJ
Sample : K1223-08 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-T

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-BF011619.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 | 5.063 | 502 | 506 | 514 | rVB | 62111 | 67317 | 3.07% | 0.240% |
| 2 | 5.492 | 575 | 579 | 592 | rBV | 1346394 | 1395452 | 63.68% | 4.982% |
| 3 | 6.140 | 685 | 689 | 691 | rBV | 27025 | 26288 | 1.20% | 0.094% |
| 4 | 6.504 | 747 | 751 | 759 | rBV | 1500250 | 1505336 | 68.69% | 5.375% |
| 5 | 6.634 | 769 | 773 | 781 | rVB | 1802796 | 1595982 | 72.83% | 5.698% |
| 6 | 6.857 | 807 | 811 | 818 | rBV | 1142424 | 940066 | 42.90% | 3.356% |
| 7 | 7.010 | 834 | 837 | 845 | rVB | 1382170 | 1235994 | 56.40% | 4.413% |
| 8 | 7.416 | 902 | 906 | 915 | rBV | 1010670 | 911707 | 41.60% | 3.255% |
| 9 | 8.139 | 1025 | 1029 | 1032 | rBV | 1446654 | 1195424 | 54.55% | 4.268% |
| 10 | 9.210 | 1208 | 1211 | 1221 | rBV | 2467557 | 2191499 | 100.00% | 7.825% |
| 11 | 9.292 | 1221 | 1225 | 1227 | rVV2 | 29227 | 41096 | 1.88% | 0.147% |
| 12 | 9.328 | 1227 | 1231 | 1234 | rVV2 | 110180 | 108755 | 4.96% | 0.388% |
| 13 | 9.363 | 1234 | 1237 | 1243 | rVB4 | 35995 | 58713 | 2.68% | 0.210% |
| 14 | 9.527 | 1263 | 1265 | 1267 | rBV2 | 53456 | 52362 | 2.39% | 0.187% |
| 15 | 9.551 | 1267 | 1269 | 1273 | rVV | 366417 | 339923 | 15.51% | 1.214% |
| 16 | 9.604 | 1275 | 1278 | 1282 | rVB | 201066 | 190113 | 8.68% | 0.679% |
| 17 | 9.651 | 1282 | 1286 | 1288 | rBV | 116077 | 96175 | 4.39% | 0.343% |
| 18 | 9.804 | 1310 | 1312 | 1317 | rVB4 | 41874 | 47453 | 2.17% | 0.169% |
| 19 | 9.898 | 1324 | 1328 | 1331 | rBV | 1756908 | 1661174 | 75.80% | 5.931% |
| 20 | 9.922 | 1331 | 1332 | 1336 | rVB2 | 123962 | 83668 | 3.82% | 0.299% |
| 21 | 9.969 | 1337 | 1340 | 1343 | rVB3 | 46820 | 47969 | 2.19% | 0.171% |
| 22 | 10.016 | 1343 | 1348 | 1352 | rBV3 | 242857 | 289039 | 13.19% | 1.032% |
| 23 | 10.098 | 1359 | 1362 | 1365 | rBV2 | 57563 | 55930 | 2.55% | 0.200% |
| 24 | 10.186 | 1375 | 1377 | 1380 | rBV | 73370 | 57869 | 2.64% | 0.207% |
| 25 | 10.322 | 1394 | 1400 | 1402 | rBV4 | 29544 | 49479 | 2.26% | 0.177% |
| 26 | 10.445 | 1418 | 1421 | 1423 | rBV | 44174 | 42207 | 1.93% | 0.151% |
| 27 | 10.539 | 1434 | 1437 | 1439 | rBV2 | 84696 | 74718 | 3.41% | 0.267% |
| 28 | 10.569 | 1439 | 1442 | 1444 | rVB | 116557 | 95621 | 4.36% | 0.341% |
| 29 | 10.592 | 1444 | 1446 | 1448 | rBV2 | 24994 | 24745 | 1.13% | 0.088% |
| 30 | 10.616 | 1448 | 1450 | 1453 | rVB3 | 44616 | 40537 | 1.85% | 0.145% |
| 31 | 10.651 | 1453 | 1456 | 1459 | rBV3 | 41487 | 65221 | 2.98% | 0.233% |
| 32 | 10.686 | 1459 | 1462 | 1466 | rBV | 1337760 | 1184473 | 54.05% | 4.229% |
| 33 | 10.751 | 1471 | 1473 | 1476 | rVB | 53317 | 46600 | 2.13% | 0.166% |
| 34 | 10.804 | 1478 | 1482 | 1489 | rVB3 | 95158 | 119177 | 5.44% | 0.426% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112220.D
Acq On : 24 Jan 2019 20:29
Operator : JU/SJ
Sample : K1223-08 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-T

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-BF011619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 11.045 | 1520 | 1523 | 1525 | rBV4 | 36568 | 34745 | 1.59% | 0.124% |
| 36 | 11.098 | 1530 | 1532 | 1534 | rVV2 | 34581 | 29457 | 1.34% | 0.105% |
| 37 | 11.386 | 1575 | 1581 | 1583 | rBV | 1633841 | 1553513 | 70.89% | 5.547% |
| 38 | 11.404 | 1583 | 1584 | 1587 | rVV | 446141 | 392672 | 17.92% | 1.402% |
| 39 | 11.433 | 1587 | 1589 | 1591 | rVV | 193304 | 170485 | 7.78% | 0.609% |
| 40 | 11.457 | 1591 | 1593 | 1596 | rVV | 112557 | 102109 | 4.66% | 0.365% |
| 41 | 11.516 | 1600 | 1603 | 1606 | rVB | 140042 | 128122 | 5.85% | 0.457% |
| 42 | 11.598 | 1613 | 1617 | 1619 | rBV3 | 74851 | 97923 | 4.47% | 0.350% |
| 43 | 11.669 | 1627 | 1629 | 1633 | rBV5 | 25133 | 29100 | 1.33% | 0.104% |
| 44 | 11.727 | 1636 | 1639 | 1642 | rVV | 121705 | 115476 | 5.27% | 0.412% |
| 45 | 11.763 | 1643 | 1645 | 1648 | rVB2 | 59732 | 59300 | 2.71% | 0.212% |
| 46 | 11.827 | 1654 | 1656 | 1659 | rBV4 | 31940 | 36388 | 1.66% | 0.130% |
| 47 | 11.869 | 1659 | 1663 | 1667 | rBV | 300997 | 324173 | 14.79% | 1.157% |
| 48 | 11.910 | 1667 | 1670 | 1677 | rVV2 | 410834 | 456129 | 20.81% | 1.629% |
| 49 | 11.998 | 1682 | 1685 | 1687 | rBV | 55641 | 57626 | 2.63% | 0.206% |
| 50 | 12.080 | 1693 | 1699 | 1702 | rBV3 | 184475 | 245674 | 11.21% | 0.877% |
| 51 | 12.157 | 1710 | 1712 | 1714 | rBV | 44028 | 48158 | 2.20% | 0.172% |
| 52 | 12.269 | 1728 | 1731 | 1733 | rVB3 | 76728 | 55860 | 2.55% | 0.199% |
| 53 | 12.304 | 1735 | 1737 | 1739 | rBV2 | 60298 | 63365 | 2.89% | 0.226% |
| 54 | 12.357 | 1744 | 1746 | 1749 | rBV3 | 64435 | 63520 | 2.90% | 0.227% |
| 55 | 12.421 | 1754 | 1757 | 1759 | rBV | 186855 | 203028 | 9.26% | 0.725% |
| 56 | 12.451 | 1759 | 1762 | 1764 | rVV4 | 122706 | 162319 | 7.41% | 0.580% |
| 57 | 12.474 | 1764 | 1766 | 1769 | rVV2 | 194058 | 155920 | 7.11% | 0.557% |
| 58 | 12.516 | 1770 | 1773 | 1778 | rBV | 579675 | 575962 | 26.28% | 2.056% |
| 59 | 12.598 | 1784 | 1787 | 1797 | rBV | 586692 | 816802 | 37.27% | 2.916% |
| 60 | 12.692 | 1800 | 1803 | 1806 | rVV3 | 101852 | 101575 | 4.63% | 0.363% |
| 61 | 12.827 | 1823 | 1826 | 1832 | rVB | 440948 | 467276 | 21.32% | 1.668% |
| 62 | 12.880 | 1833 | 1835 | 1839 | rVB3 | 104207 | 96697 | 4.41% | 0.345% |
| 63 | 12.963 | 1846 | 1849 | 1853 | rBV | 1806814 | 1592031 | 72.65% | 5.684% |
| 64 | 13.398 | 1921 | 1923 | 1927 | rBV2 | 308891 | 268741 | 12.26% | 0.960% |
| 65 | 13.468 | 1933 | 1935 | 1941 | rVB | 219721 | 229506 | 10.47% | 0.819% |
| 66 | 13.857 | 1998 | 2001 | 2006 | rBV4 | 362229 | 403706 | 18.42% | 1.441% |
| 67 | 14.027 | 2026 | 2030 | 2033 | rBV2 | 1192613 | 1260633 | 57.52% | 4.501% |
| 68 | 14.868 | 2170 | 2173 | 2176 | rVB | 495634 | 503321 | 22.97% | 1.797% |
| 69 | 15.133 | 2215 | 2218 | 2220 | rBV | 347622 | 358741 | 16.37% | 1.281% |
| 70 | 15.509 | 2279 | 2282 | 2286 | rVB | 681571 | 809884 | 36.96% | 2.892% |

LSC Area Percent Report

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Acq On : 24 Jan 2019 20:29
Operator : JU/SJ
Sample : K1223-08 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TS-T

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-BF011619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 28008019

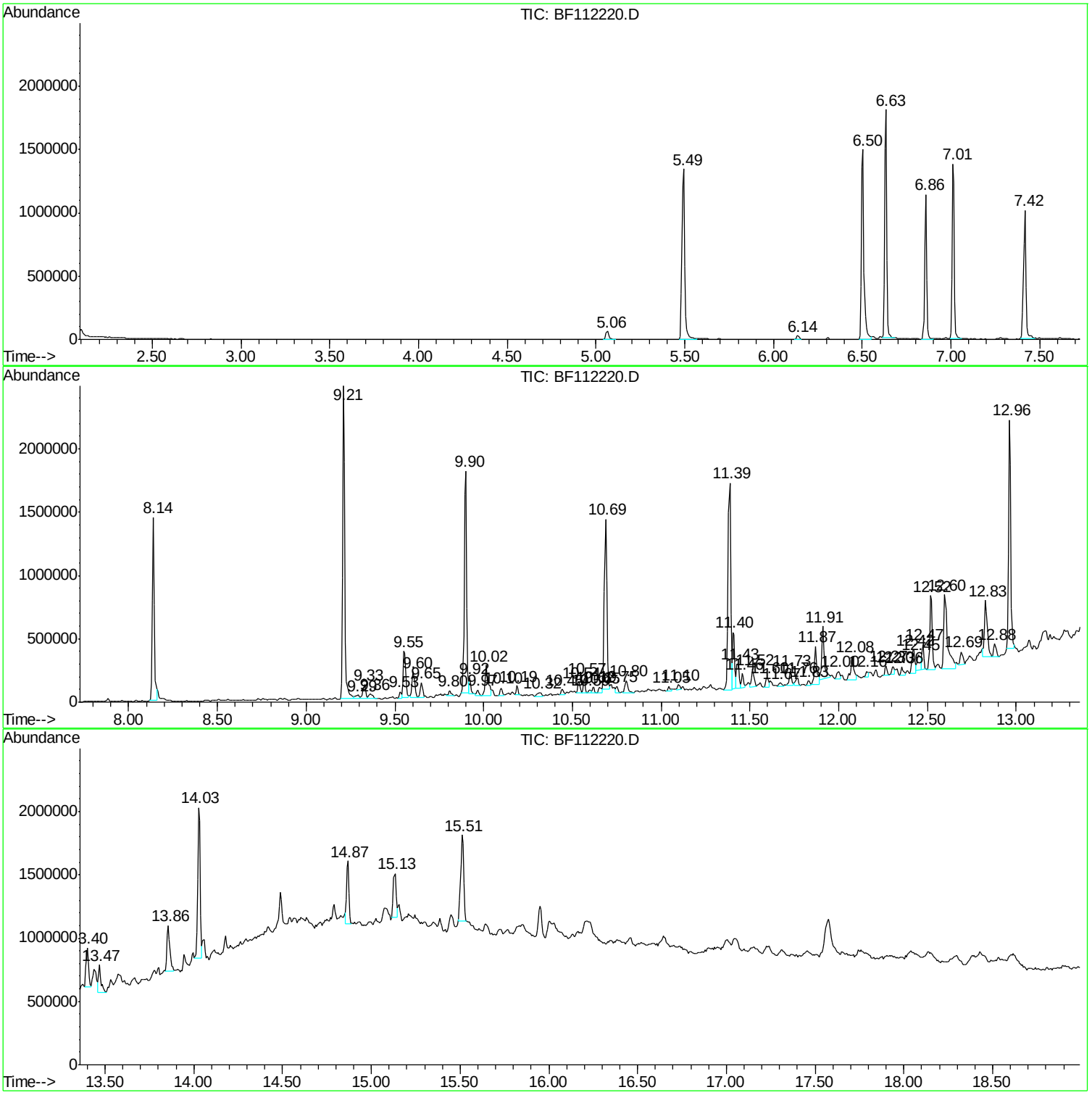
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112220.D
Acq On : 24 Jan 2019 20:29
Operator : JU/SJ
Sample : K1223-08 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TS-T

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.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\BF012419\
Data File : BF112220.D
Acq On : 24 Jan 2019 20:29
Operator : JU/SJ
Sample : K1223-08 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-T

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

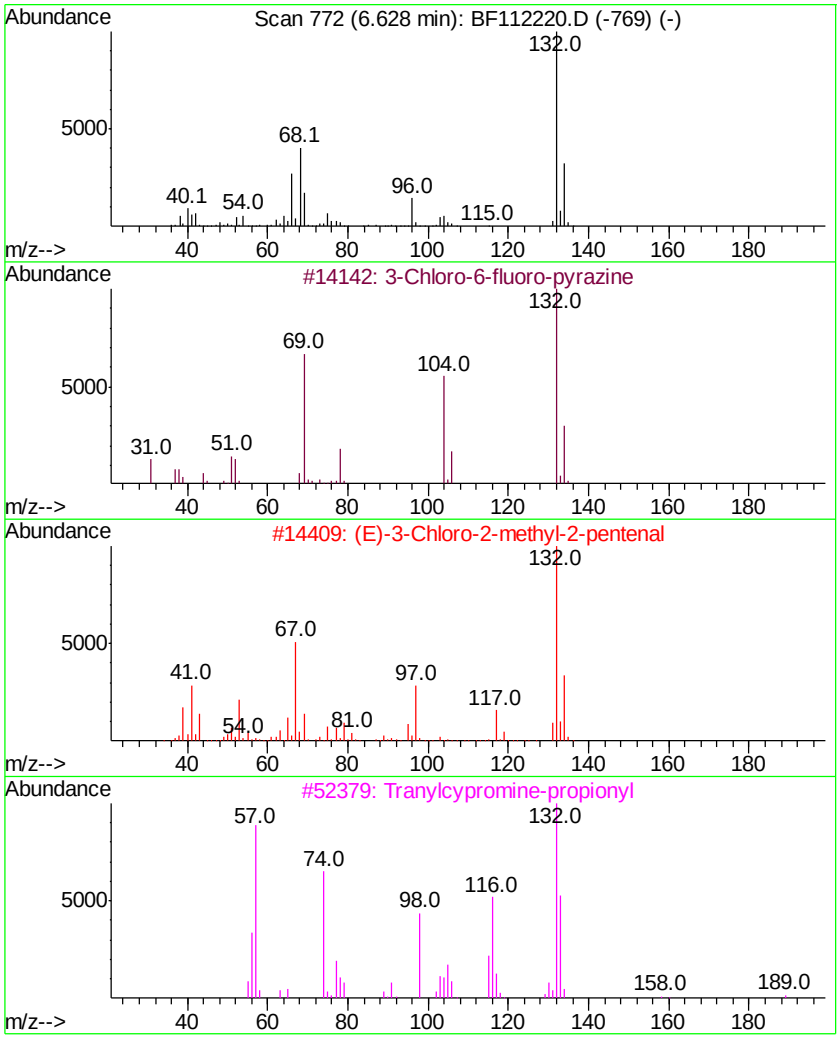
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

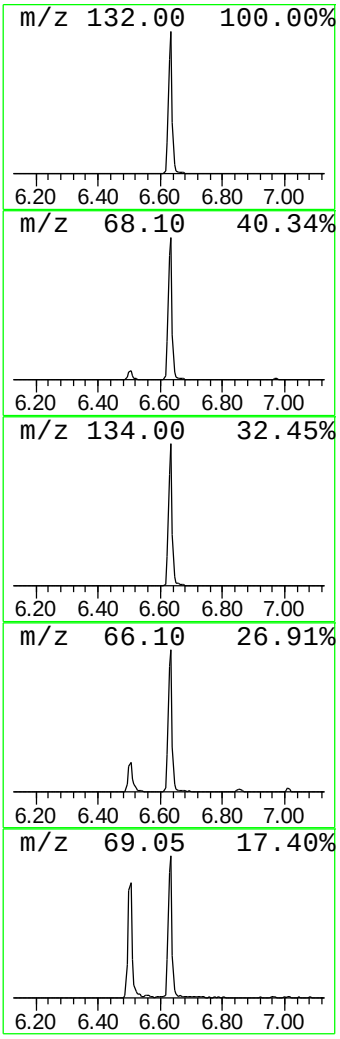
**********

Peak Number 1 unknown6.63 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.63 | 33.95 ng | 1595980 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 25 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 17 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 16 |
| 4 | 1-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-59-9 | 9 |
| 5 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112220.D
Acq On : 24 Jan 2019 20:29
Operator : JU/SJ
Sample : K1223-08 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-T

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

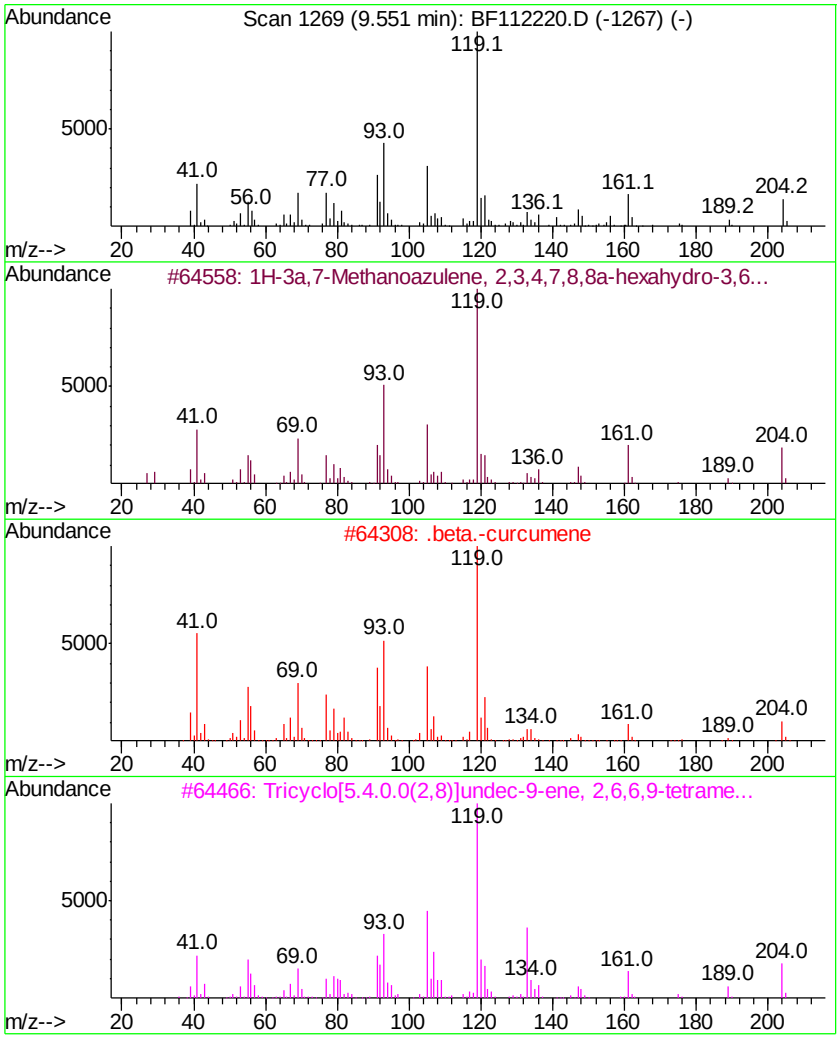
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

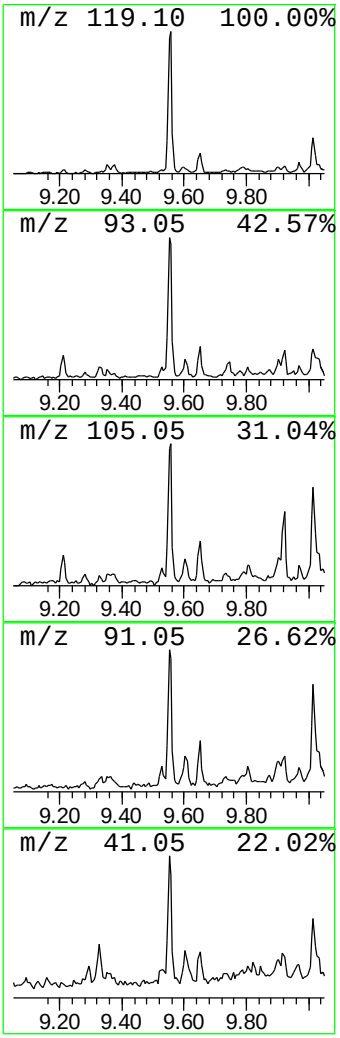
**********

Peak Number 3 1H-3a,7-Methanoazulene, 2,3... Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.55 | 4.09 ng | 339923 | Acenaphthene-d10 | 9.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1H-3a,7-Methanoazulene, 2,3,4,7,... | 204 | C15H24 | 000469-61-4 | 99 |
| 2 | .beta.-curcumene | 204 | C15H24 | 1000374-17-4 | 87 |
| 3 | Tricyclo[5.4.0.0(2,8)]undec-9-en... | 204 | C15H24 | 005989-08-2 | 59 |
| 4 | Copaene | 204 | C15H24 | 003856-25-5 | 43 |
| 5 | Benzene, 1-(1,5-dimethylhexyl)-4... | 204 | C15H24 | 001461-02-5 | 43 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112220.D
Acq On : 24 Jan 2019 20:29
Operator : JU/SJ
Sample : K1223-08 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-T

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

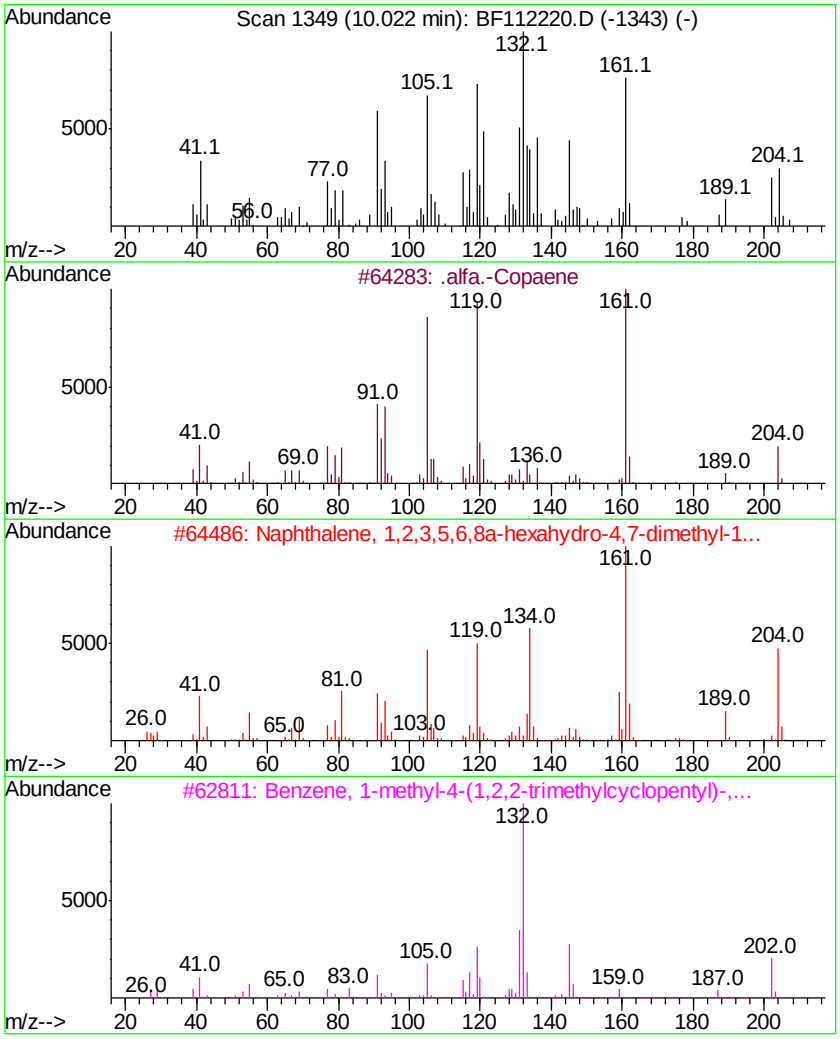
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

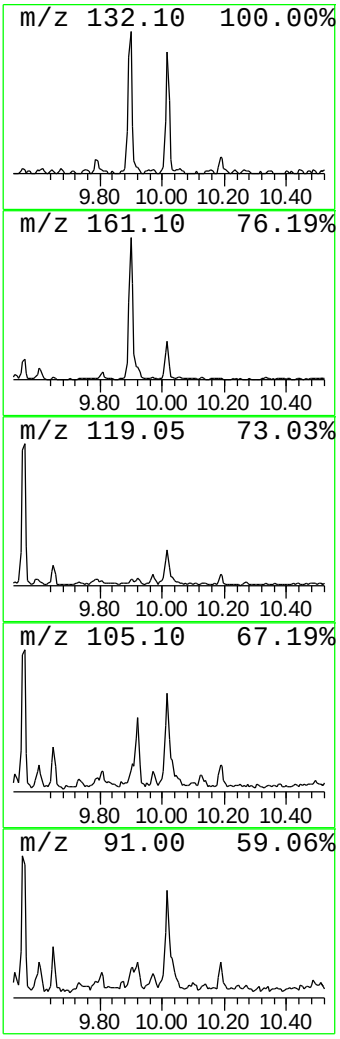
**********

Peak Number 4 .alfa.-Copaene Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.02 | 3.48 ng | 289039 | Acenaphthene-d10 | 9.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | .alfa.-Copaene | 204 | C15H24 | 1000360-33-0 | 86 |
| 2 | Naphthalene, 1,2,3,5,6,8a-hexahy... | 204 | C15H24 | 000483-76-1 | 62 |
| 3 | Benzene, 1-methyl-4-(1,2,2-trime... | 202 | C15H22 | 016982-00-6 | 55 |
| 4 | Benzene, 1-(1,5-dimethyl-4-hexen... | 202 | C15H22 | 000644-30-4 | 50 |
| 5 | .gamma.-Muurolene | 204 | C15H24 | 030021-74-0 | 50 |



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**Instrument :** BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

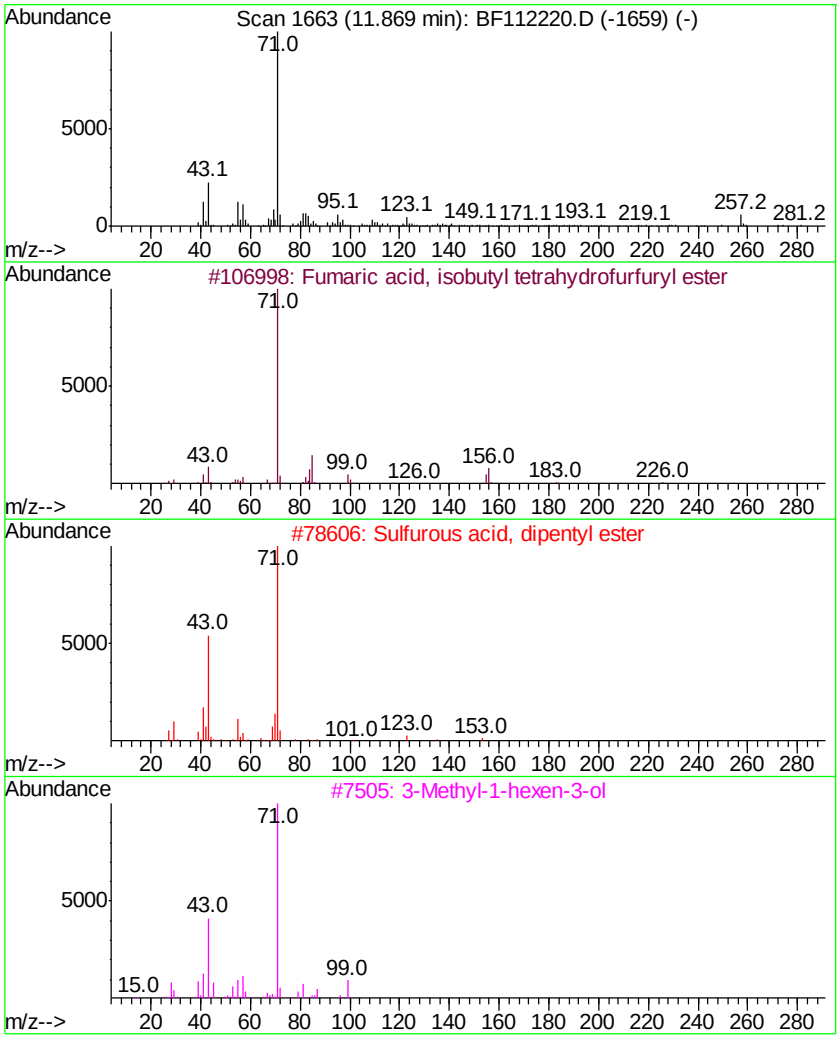
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

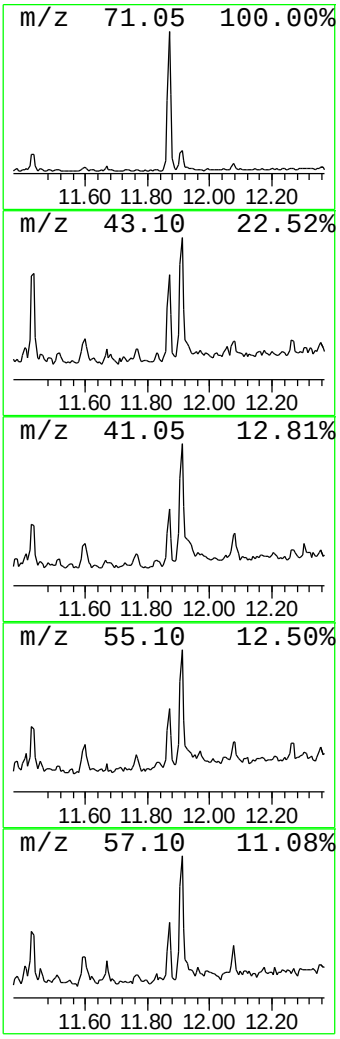
**********

Peak Number 5 Fumaric acid, isobutyl tetr... Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.87 | 4.17 ng | 324173 | Phenanthrene-d10 | 11.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Fumaric acid, isobutyl tetrahydr... | 256 | C13H20O5 | 1000330-57-8 | 59 |
| 2 | Sulfurous acid, dipentyl ester | 222 | C10H22O3S | 1000309-13-9 | 59 |
| 3 | 3-Methyl-1-hexen-3-ol | 114 | C7H14O | 055145-28-3 | 59 |
| 4 | Valeric acid, 2-tetrahydrofurylm... | 186 | C10H18O3 | 005451-86-5 | 59 |
| 5 | 3-Cyclopentylpropionic acid, 2-t... | 226 | C13H22O3 | 1000293-46-9 | 53 |



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Acq On : 24 Jan 2019 20:29
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Sample : K1223-08 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-T

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

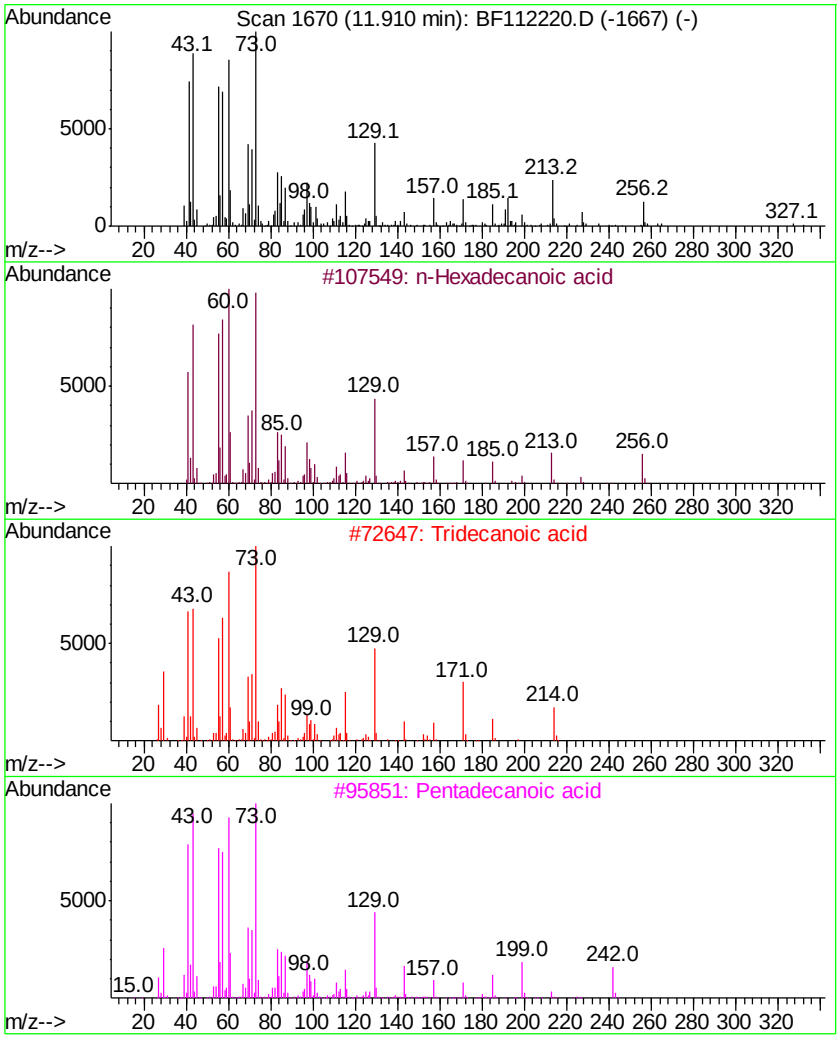
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

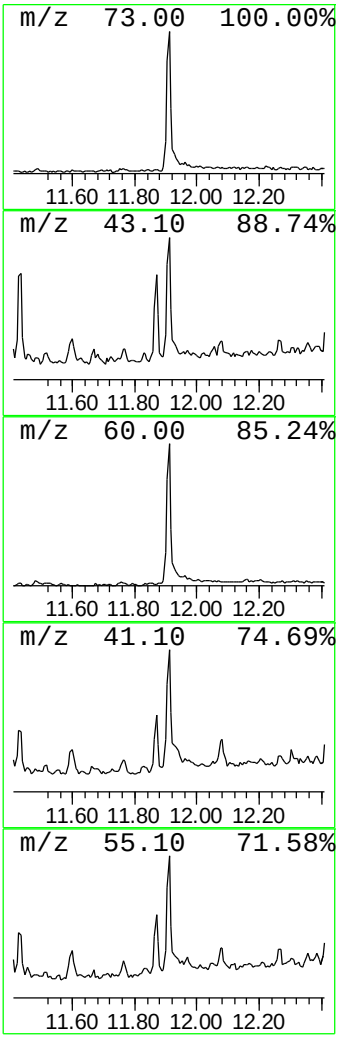
**********

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.91 | 5.87 ng | 456129 | Phenanthrene-d10 | 11.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 95 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 91 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 90 |
| 5 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 81 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112220.D
Acq On : 24 Jan 2019 20:29
Operator : JU/SJ
Sample : K1223-08 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-T

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

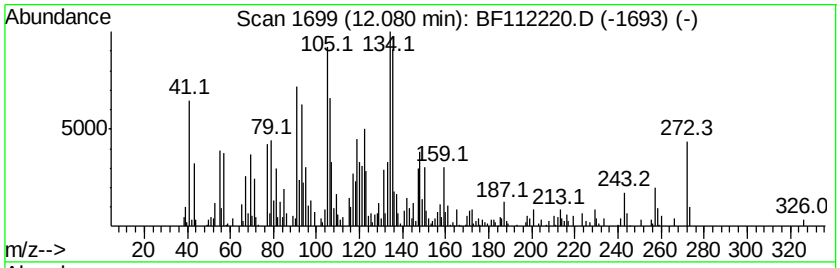
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

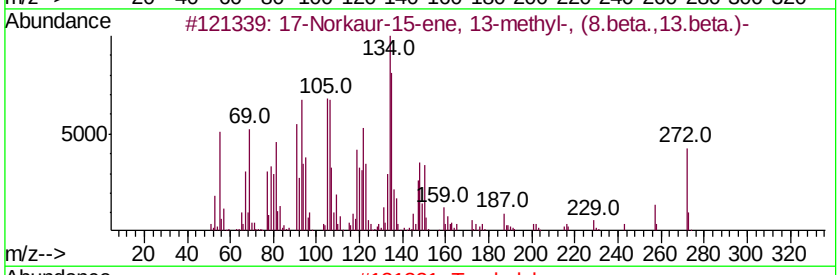
**********

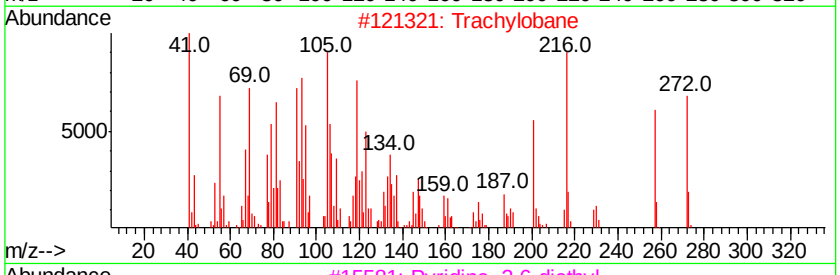
Peak Number 7 17-Norkaur-15-ene, 13-methy... Concentration Rank 13

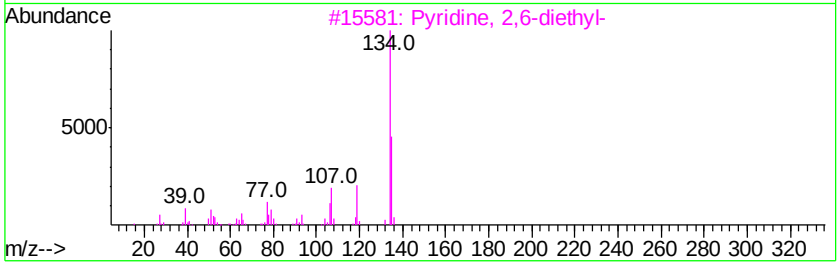
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.08 | 3.16 ng | 245674 | Phenanthrene-d10 | 11.39 |

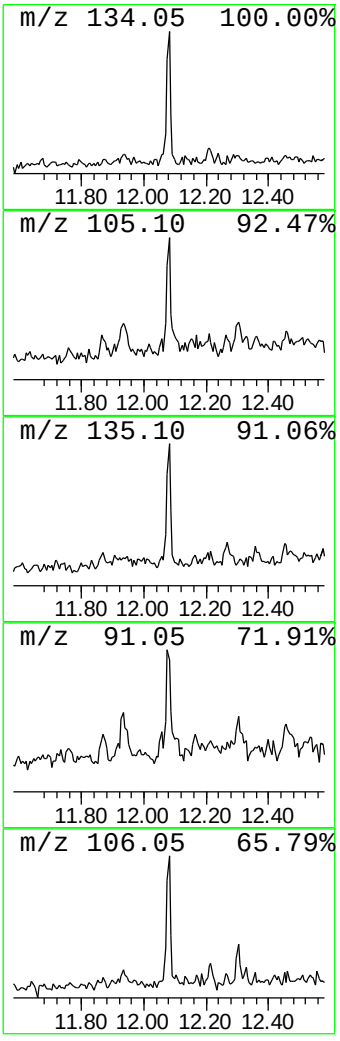
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 17-Norkaur-15-ene, 13-methyl-, (... | 272 | C20H32 | 003564-54-3 | 93 |
| 2 | Trachylobane | 272 | C20H32 | 005282-35-9 | 30 |
| 3 | Pyridine, 2,6-diethyl- | 135 | C9H13N | 000935-28-4 | 22 |
| 4 | 2-Allylphenol | 134 | C9H10O | 001745-81-9 | 18 |
| 5 | Formamide, N-(2-methylphenyl)- | 135 | C8H9NO | 000094-69-9 | 18 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112220.D
Acq On : 24 Jan 2019 20:29
Operator : JU/SJ
Sample : K1223-08 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-T

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

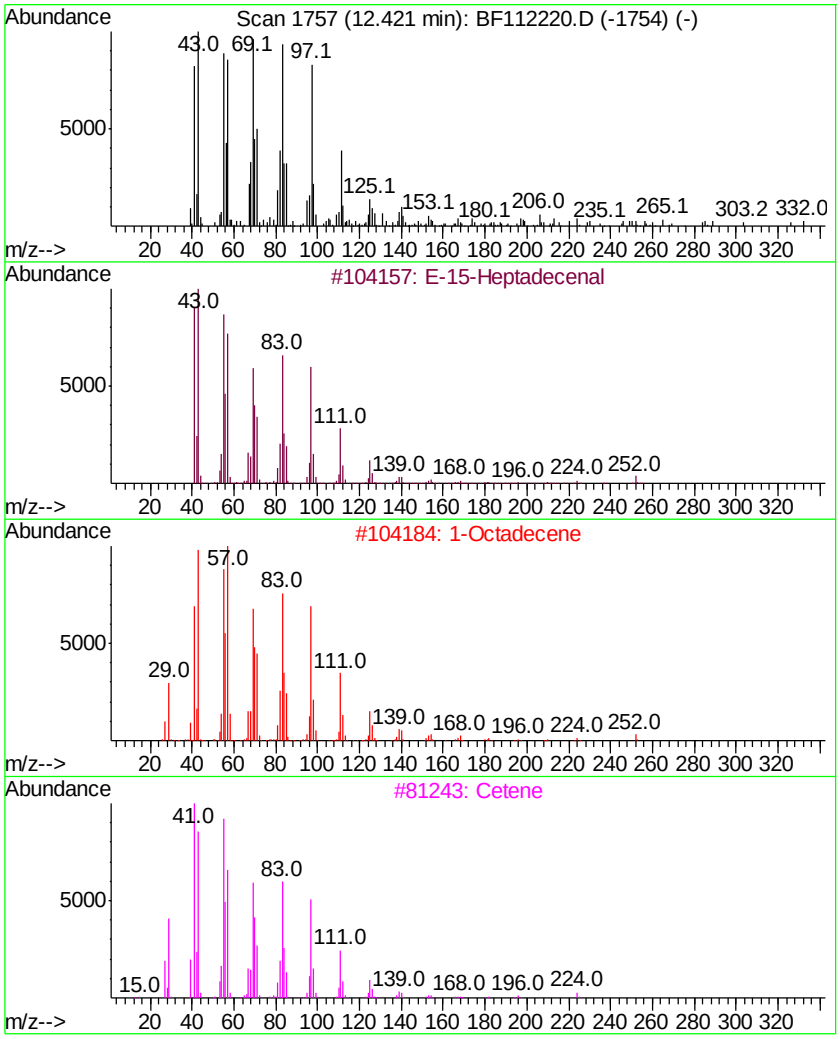
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

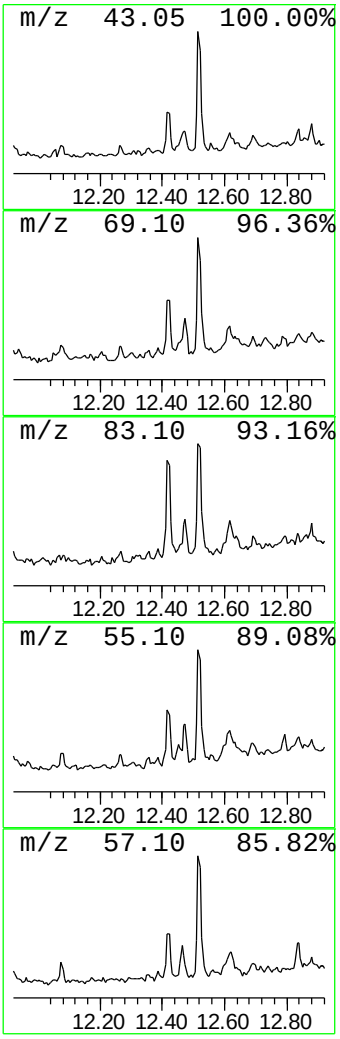
**********

Peak Number 8 E-15-Heptadecenal Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.42 | 2.61 ng | 203028 | Phenanthrene-d10 | 11.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | E-15-Heptadecenal | 252 | C17H32O | 1000130-97-9 | 98 |
| 2 | 1-Octadecene | 252 | C18H36 | 000112-88-9 | 95 |
| 3 | Cetene | 224 | C16H32 | 000629-73-2 | 95 |
| 4 | 1-Hexadecanol | 242 | C16H34O | 036653-82-4 | 93 |
| 5 | Bromoacetic acid, octadecyl ester | 390 | C20H39BrO2 | 018992-03-5 | 91 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112220.D
Acq On : 24 Jan 2019 20:29
Operator : JU/SJ
Sample : K1223-08 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-T

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

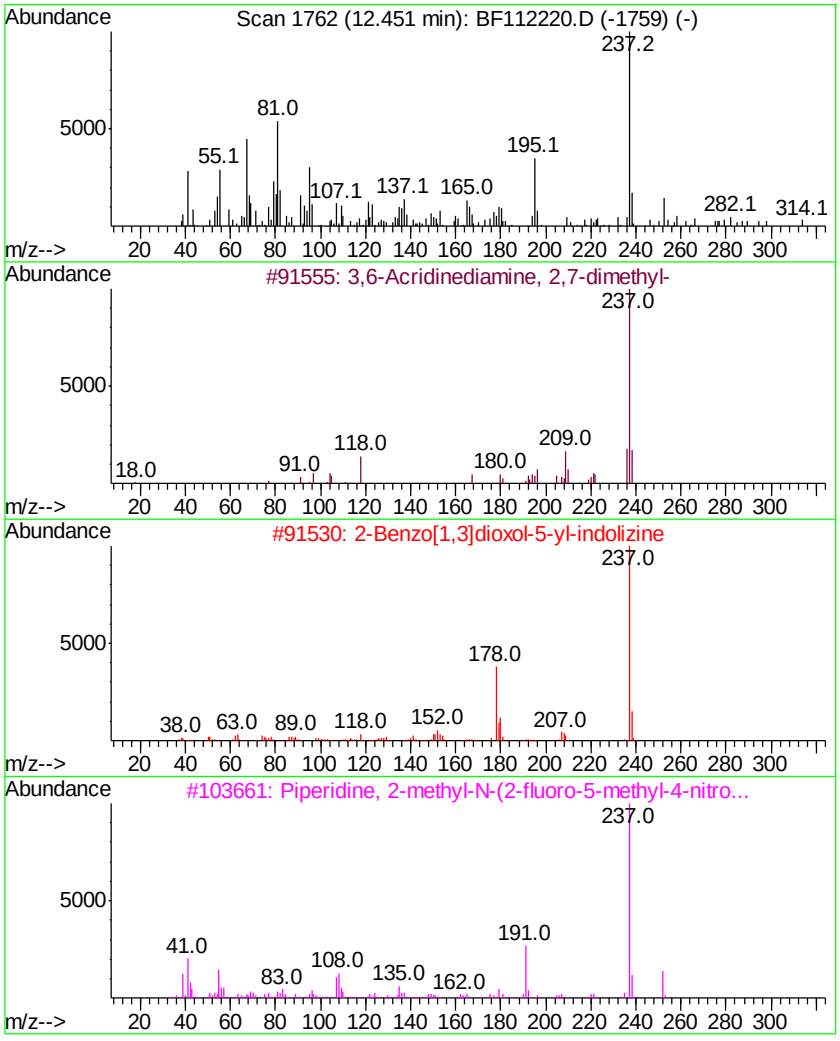
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

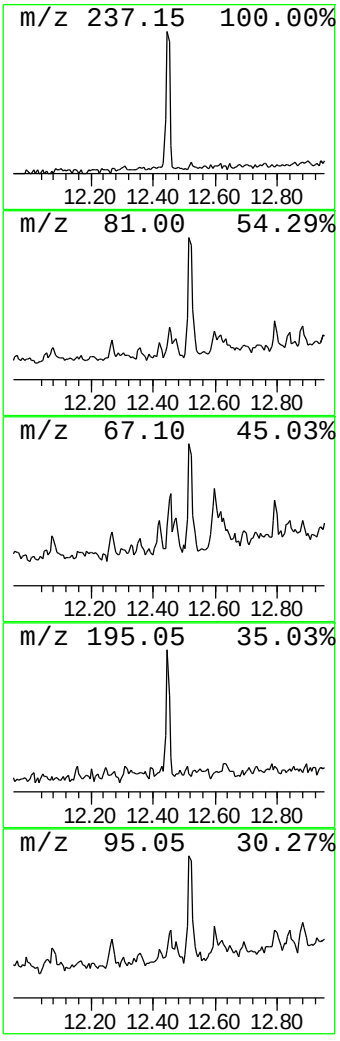
**********

Peak Number 9 unknown12.45 Concentration Rank 15

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.45 | 2.09 ng | 162319 | Phenanthrene-d10 | 11.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3,6-Acridinediamine, 2,7-dimethyl- | 237 | C15H15N3 | 000092-26-2 | 49 |
| 2 | 2-Benzo[1,3]dioxol-5-yl-indolizine | 237 | C15H11NO2 | 1000301-42-4 | 46 |
| 3 | Piperidine, 2-methyl-N-(2-fluoro... | 252 | C13H17FN2O2 | 1000277-62-4 | 43 |
| 4 | 3,5-Dimethyl-1-[4-(1H-pyrrol-1-y... | 237 | C15H15N3 | 257863-12-0 | 43 |
| 5 | 8-Dimethylamino-1,3,7-trimethyl-... | 237 | C10H15N5O2 | 078146-62-0 | 40 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112220.D
Acq On : 24 Jan 2019 20:29
Operator : JU/SJ
Sample : K1223-08 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-T

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

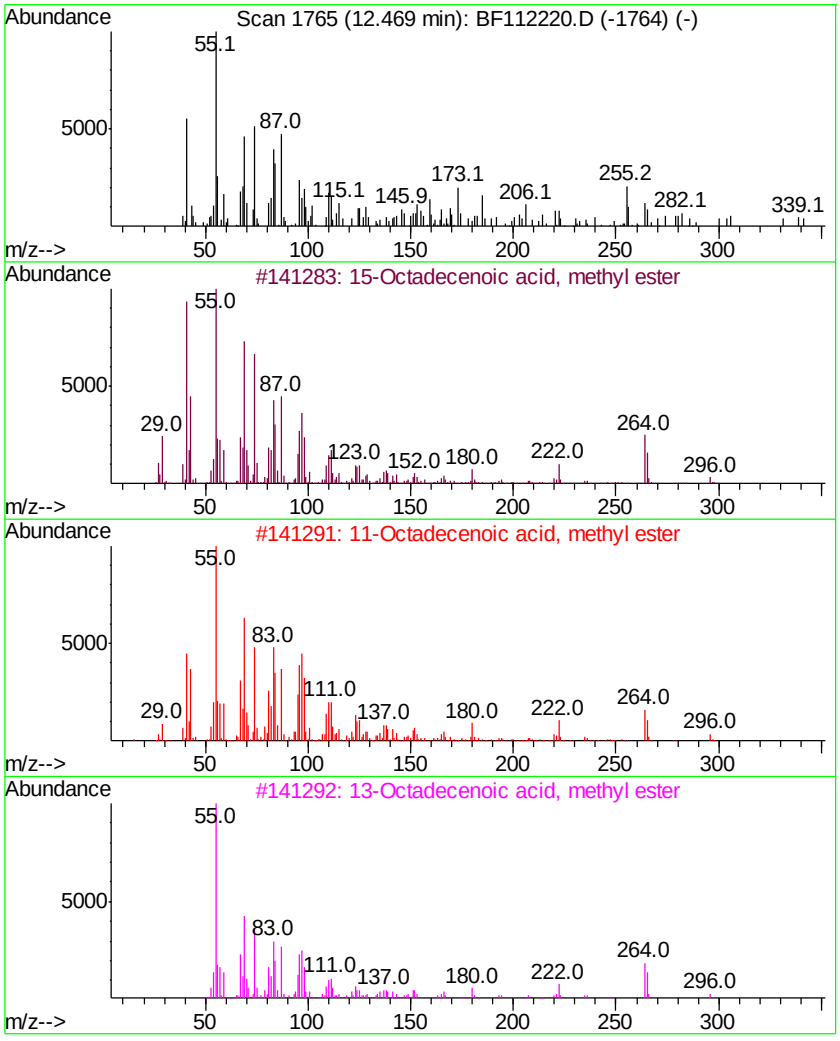
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

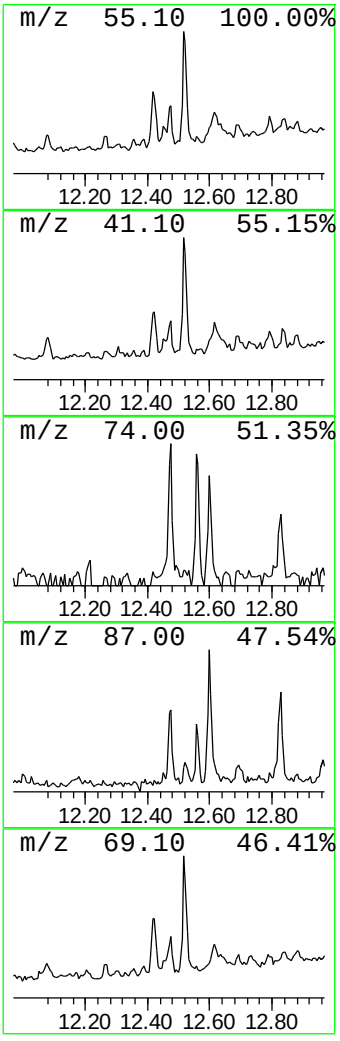
**********

Peak Number 10 15-Octadecenoic acid, methy... Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.47 | 2.01 ng | 155920 | Phenanthrene-d10 | 11.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 15-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 004764-72-1 | 95 |
| 2 | 11-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 052380-33-3 | 86 |
| 3 | 13-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 056554-47-3 | 84 |
| 4 | 14-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 056554-48-4 | 80 |
| 5 | 8-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 002345-29-1 | 70 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112220.D
Acq On : 24 Jan 2019 20:29
Operator : JU/SJ
Sample : K1223-08 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-T

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

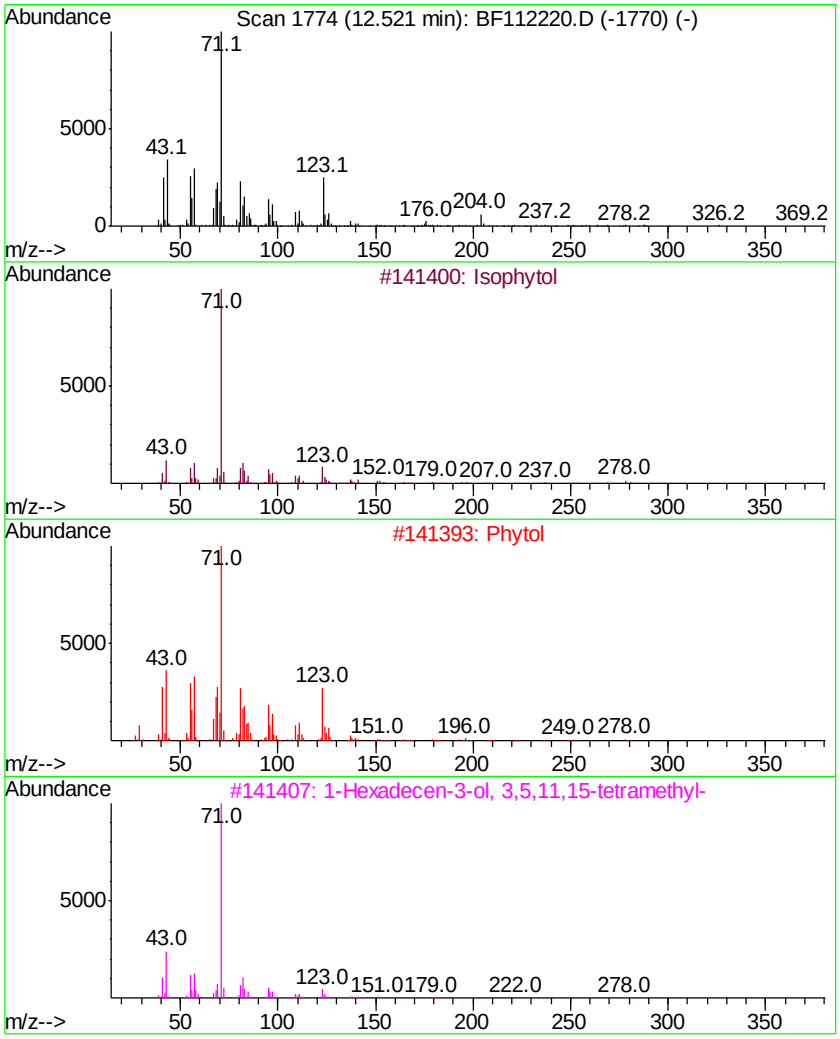
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

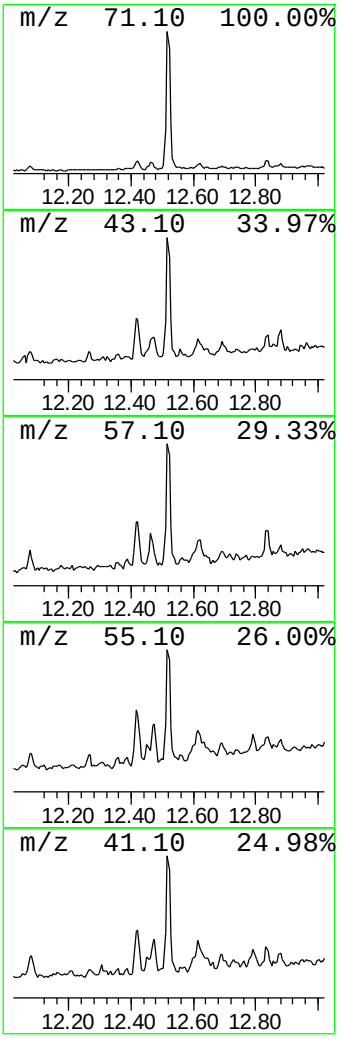
**********

Peak Number 11 Isophytol Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.52 | 7.41 ng | 575962 | Phenanthrene-d10 | 11.39 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Isophytol | 296 | C20H40O | 000505-32-8 | 72 |
| 2 | Phytol | 296 | C20H40O | 000150-86-7 | 70 |
| 3 | 1-Hexadecen-3-ol, 3,5,11,15-tetr... | 296 | C20H40O | 1000262-55-5 | 59 |
| 4 | Butyric acid, 3-pentadecyl ester | 298 | C19H38O2 | 1000280-57-3 | 53 |
| 5 | Sulfurous acid, octadecyl 2-pent... | 404 | C23H48O3S | 1000309-16-6 | 50 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112220.D
Acq On : 24 Jan 2019 20:29
Operator : JU/SJ
Sample : K1223-08 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-T

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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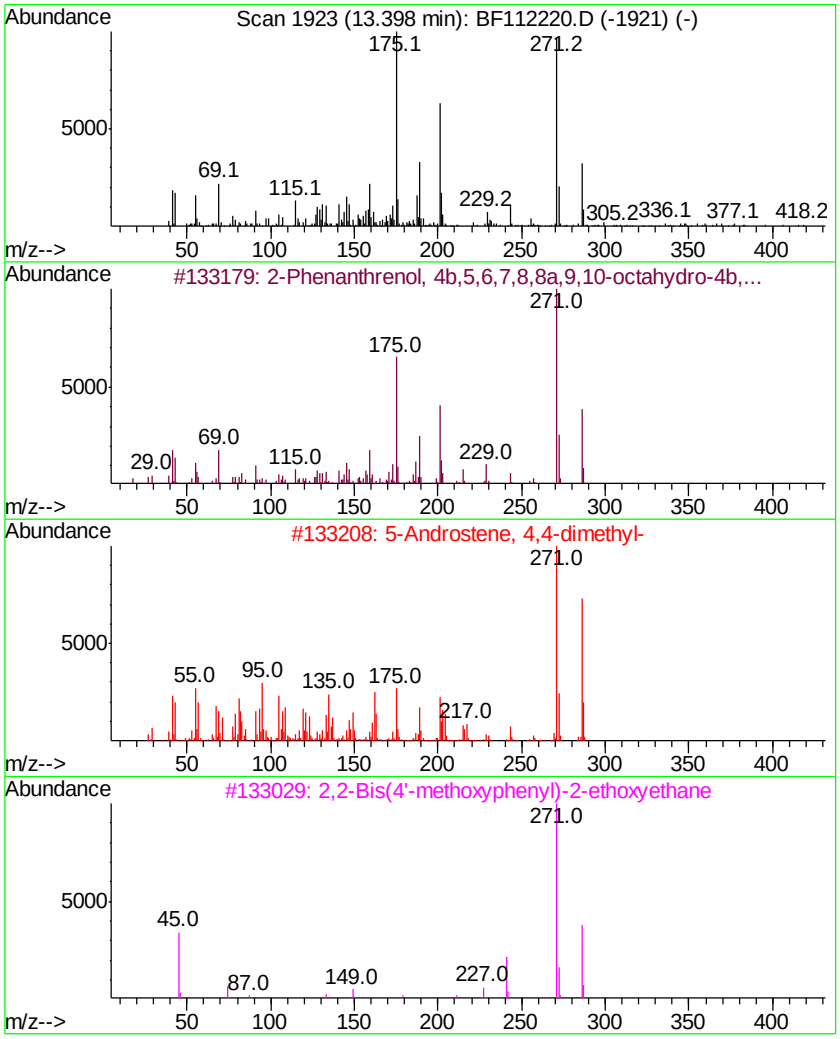
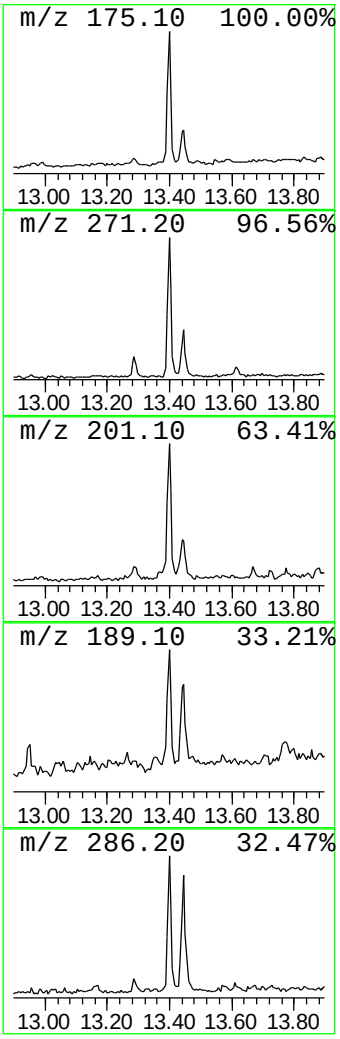
Peak Number 12 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.40 | 4.26 ng | 268741 | Chrysene-d12 | 14.03 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Phenanthrenol, 4b,5,6,7,8,8a,9... | 286 | C20H30O | 000511-15-9 | 91 |
| 2 | 5-Androstene, 4,4-dimethyl- | 286 | C21H34 | 1000194-15-4 | 53 |
| 3 | 2,2-Bis(4'-methoxyphenyl)-2-etho... | 286 | C18H22O3 | 1000283-53-7 | 27 |
| 4 | Benzene, 1,4-dimethyl-2,5-bis(1-... | 190 | C14H22 | 010375-96-9 | 14 |
| 5 | 2-(2,4-Dichloro-benzylsulfanylme... | 365 | C17H13Cl2NO2S | 1000294-87-3 | 14 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112220.D
Acq On : 24 Jan 2019 20:29
Operator : JU/SJ
Sample : K1223-08 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-T

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

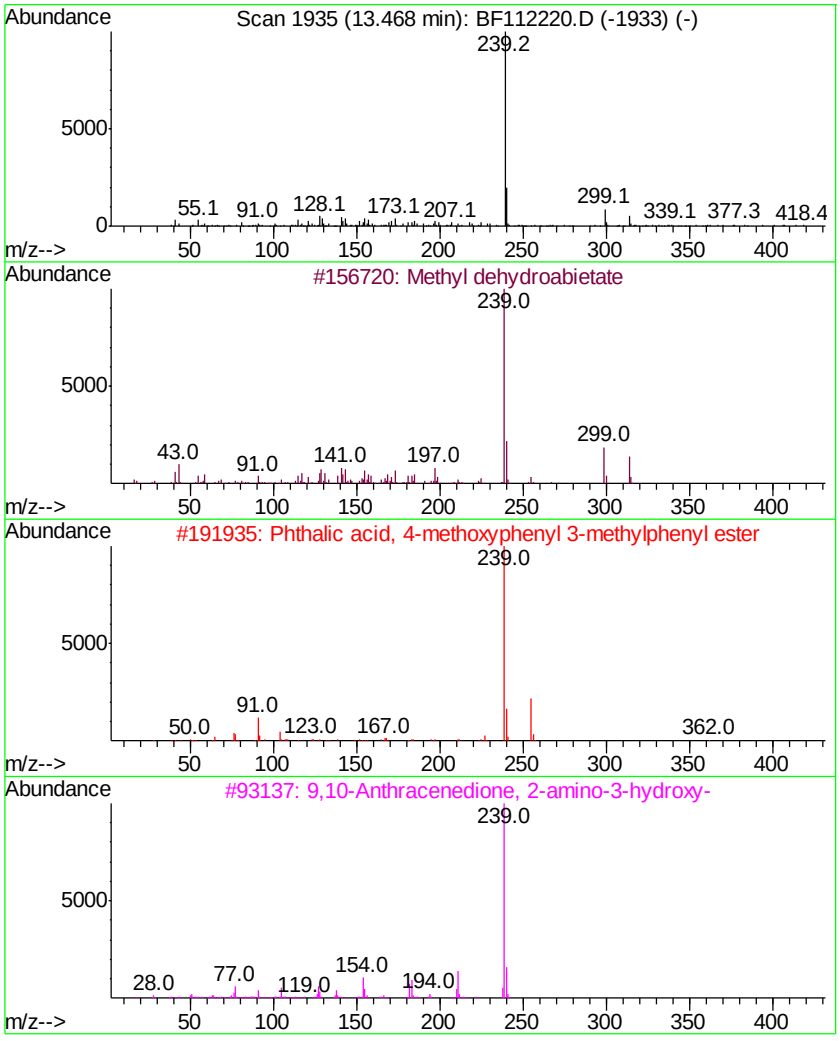
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

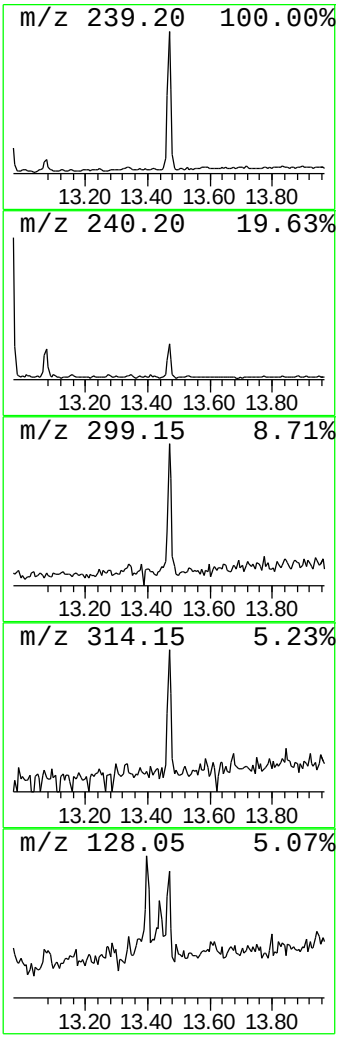
**********

Peak Number 13 Methyl dehydroabietate Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.47 | 3.64 ng | 229506 | Chrysene-d12 | 14.03 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methyl dehydroabietate | 314 | C21H30O2 | 001235-74-1 | 83 |
| 2 | Phthalic acid, 4-methoxyphenyl 3... | 362 | C22H18O5 | 1000315-68-0 | 64 |
| 3 | 9,10-Anthracenedione, 2-amino-3-... | 239 | C14H9NO3 | 000117-77-1 | 53 |
| 4 | Hexadecanoic acid, 4-nitrophenyl... | 377 | C22H35NO4 | 001492-30-4 | 50 |
| 5 | (9-Hydroxymethyl-[1,10]phenanthr... | 240 | C14H12N2O2 | 078831-36-4 | 50 |



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Data File : BF112220.D
Acq On : 24 Jan 2019 20:29
Operator : JU/SJ
Sample : K1223-08 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-T

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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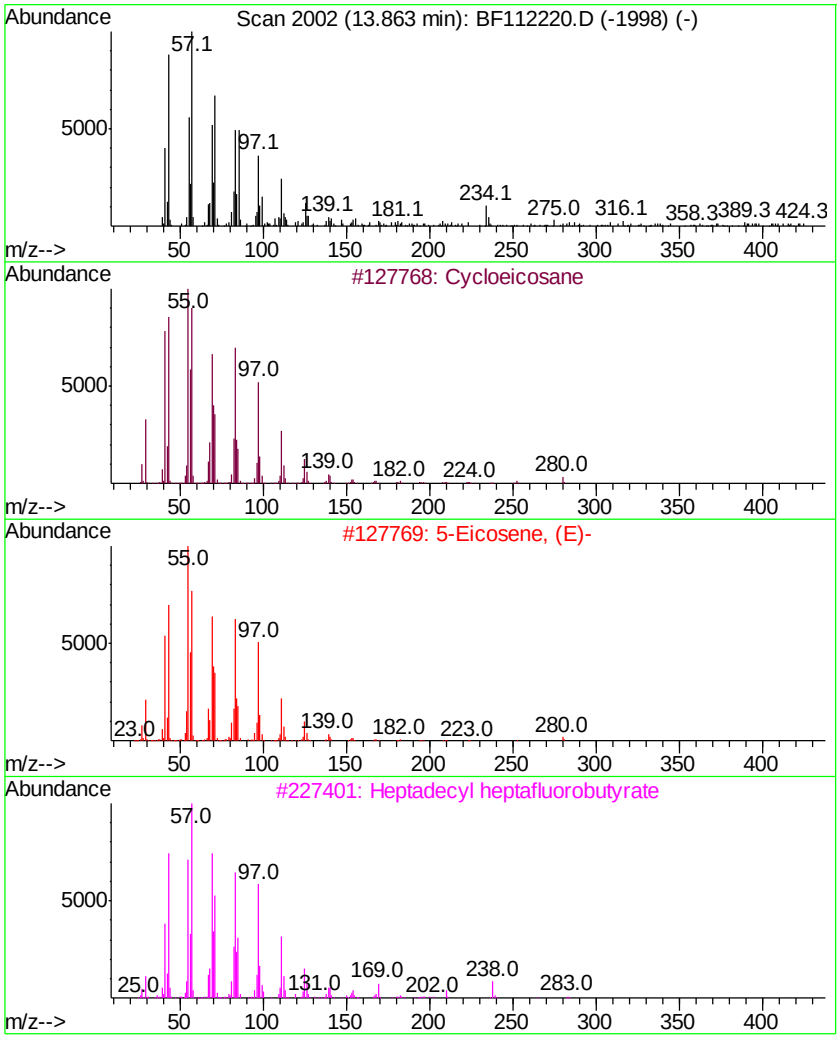
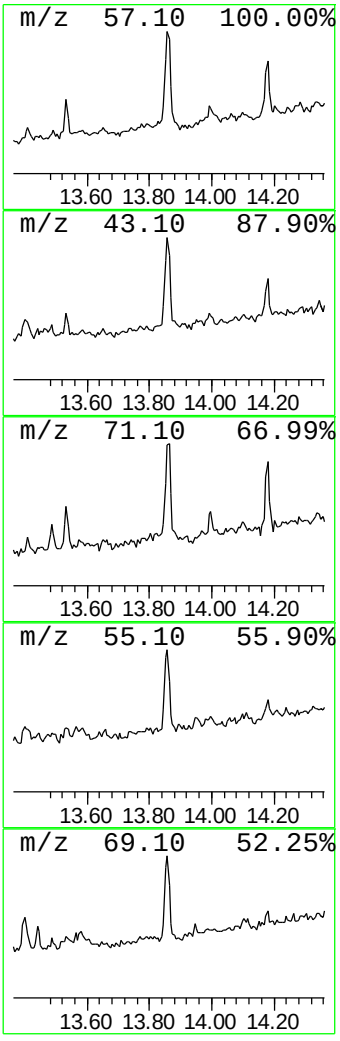
Peak Number 14 Cycloeicosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.86 | 6.40 ng | 403706 | Chrysene-d12 | 14.03 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cycloeicosane | 280 | C20H40 | 000296-56-0 | 96 |
| 2 | 5-Eicosene, (E)- | 280 | C20H40 | 074685-30-6 | 95 |
| 3 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 94 |
| 4 | 9-Tricosene, (Z)- | 322 | C23H46 | 027519-02-4 | 93 |
| 5 | Cyclopentane, (4-octyldodecyl)- | 350 | C25H50 | 005638-09-5 | 93 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112220.D
Acq On : 24 Jan 2019 20:29
Operator : JU/SJ
Sample : K1223-08 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-T

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

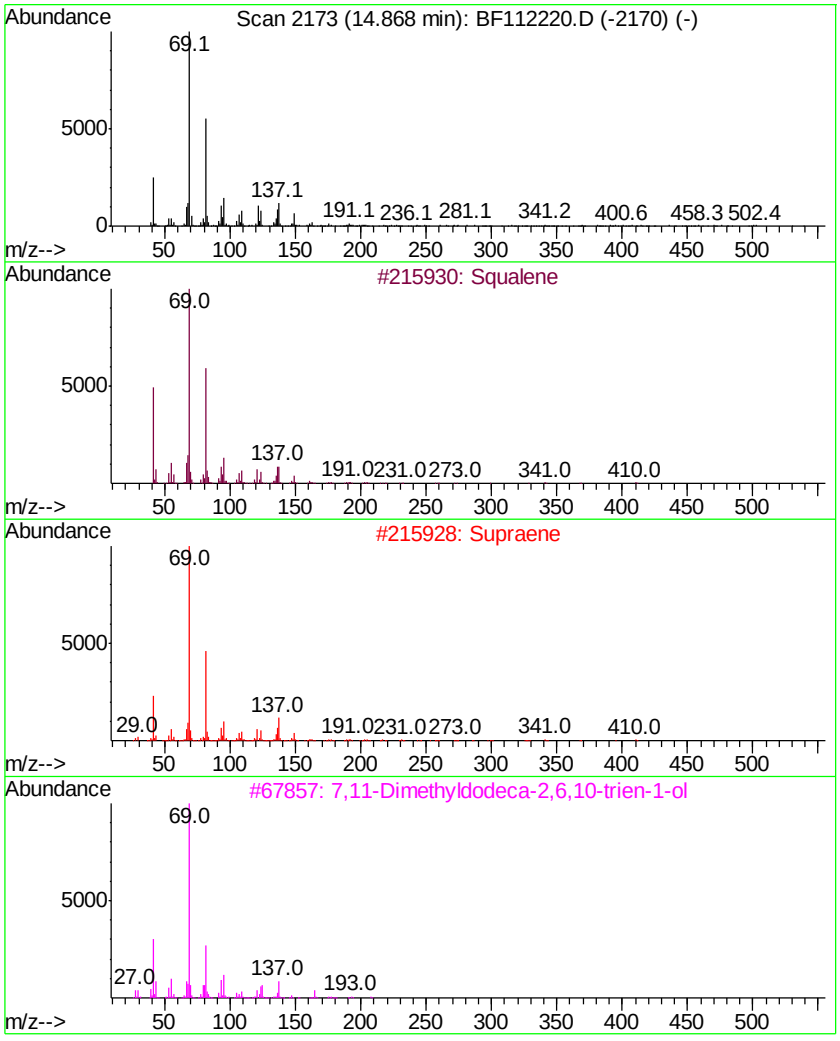
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

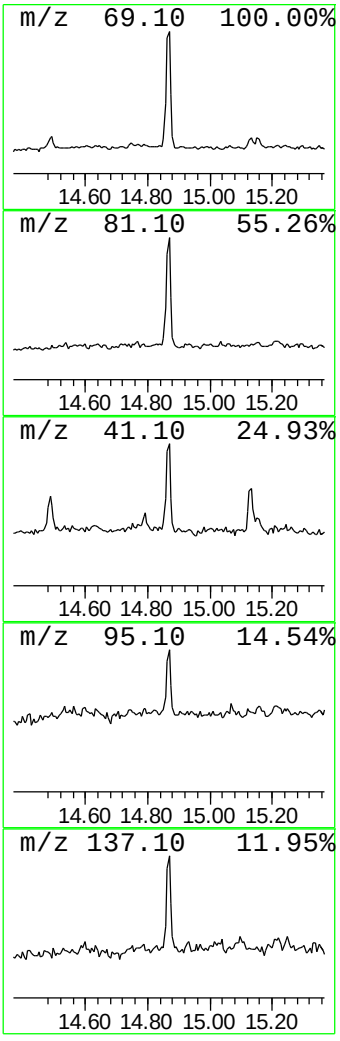
**********

Peak Number 15 Squalene Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.87 | 12.43 ng | 503321 | Perylene-d12 | 15.51 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Squalene | 410 | C30H50 | 000111-02-4 | 87 |
| 2 | Supraene | 410 | C30H50 | 007683-64-9 | 87 |
| 3 | 7,11-Dimethyldodeca-2,6,10-trien... | 208 | C14H24O | 125529-10-4 | 64 |
| 4 | trans-Geranylgeraniol | 290 | C20H34O | 024034-73-9 | 64 |
| 5 | 2,6,10,14-Hexadecatetraenoic aci... | 332 | C22H36O2 | 024035-35-6 | 59 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012419\
Data File : BF112220.D
Acq On : 24 Jan 2019 20:29
Operator : JU/SJ
Sample : K1223-08 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-T

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

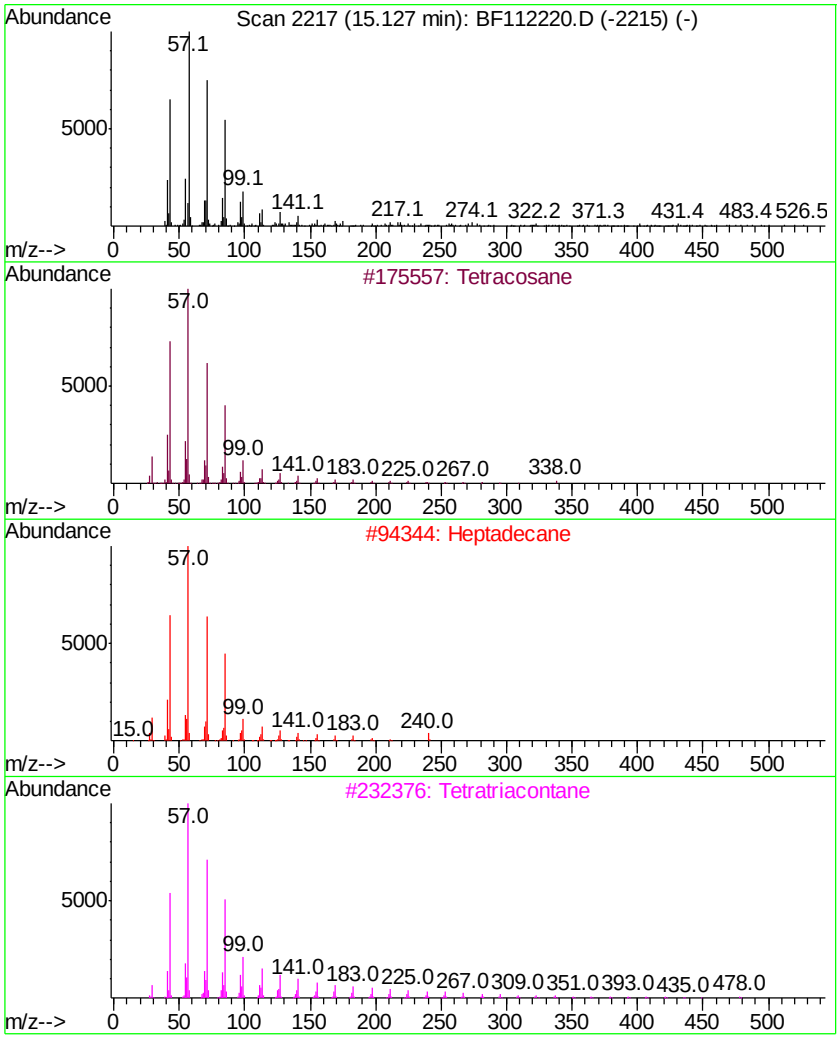
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

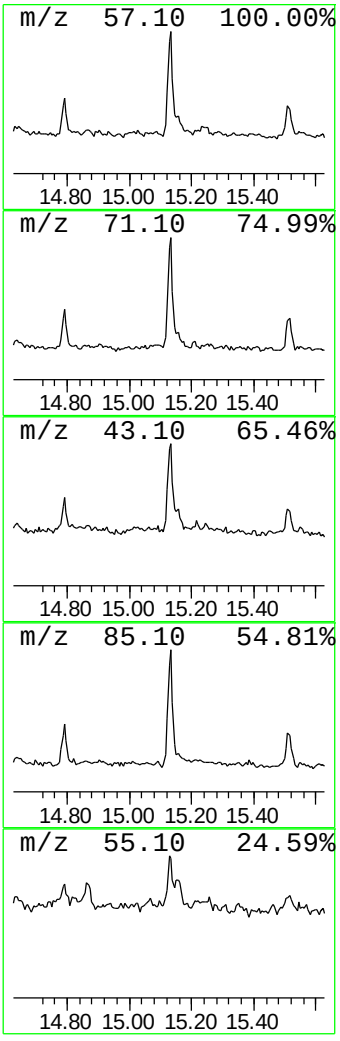
**********

Peak Number 16 Tetracosane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.13 | 8.86 ng | 358741 | Perylene-d12 | 15.51 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetracosane | 338 | C24H50 | 000646-31-1 | 93 |
| 2 | Heptadecane | 240 | C17H36 | 000629-78-7 | 93 |
| 3 | Tetratriacontane | 479 | C34H70 | 014167-59-0 | 93 |
| 4 | Heneicosane | 296 | C21H44 | 000629-94-7 | 90 |
| 5 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 90 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF012419\
Data File : BF112220.D
Acq On : 24 Jan 2019 20:29
Operator : JU/SJ
Sample : K1223-08 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** TS-T

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011619.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 |
| unknown6.63 | 6.63 | 34.0 | ng | 1595980 | 1 | 6.86 | 940066 | 20.0 |
| 1H-3a,7-Methanoaz... | 9.55 | 4.1 | ng | 339923 | 3 | 9.90 | 1661170 | 20.0 |
| .alfa.-Copaene | 10.02 | 3.5 | ng | 289039 | 3 | 9.90 | 1661170 | 20.0 |
| Fumaric acid, iso... | 11.87 | 4.2 | ng | 324173 | 4 | 11.39 | 1553510 | 20.0 |
| n-Hexadecanoic acid | 11.91 | 5.9 | ng | 456129 | 4 | 11.39 | 1553510 | 20.0 |
| 17-Norkaur-15-ene... | 12.08 | 3.2 | ng | 245674 | 4 | 11.39 | 1553510 | 20.0 |
| E-15-Heptadecenal | 12.42 | 2.6 | ng | 203028 | 4 | 11.39 | 1553510 | 20.0 |
| unknown12.45 | 12.45 | 2.1 | ng | 162319 | 4 | 11.39 | 1553510 | 20.0 |
| 15-Octadecenoic a... | 12.47 | 2.0 | ng | 155920 | 4 | 11.39 | 1553510 | 20.0 |
| Isophytol | 12.52 | 7.4 | ng | 575962 | 4 | 11.39 | 1553510 | 20.0 |
| 2-Phenanthrenol, ... | 13.40 | 4.3 | ng | 268741 | 5 | 14.03 | 1260630 | 20.0 |
| Methyl dehydroabi... | 13.47 | 3.6 | ng | 229506 | 5 | 14.03 | 1260630 | 20.0 |
| Cycloeicosane | 13.86 | 6.4 | ng | 403706 | 5 | 14.03 | 1260630 | 20.0 |
| Squalene | 14.87 | 12.4 | ng | 503321 | 6 | 15.51 | 809884 | 20.0 |
| Tetracosane | 15.13 | 8.9 | ng | 358741 | 6 | 15.51 | 809884 | 20.0 |