LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052319\
Data File : BF114552.D
Acq On : 24 May 2019 4:12
Operator : JU/SJ
Sample : K3008-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-21

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-BF051019.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 | 4.393 | 388 | 392 | 396 | rBV | 34739 | 49263 | 2.47% | 0.190% |
| 2 | 4.434 | 396 | 399 | 405 | rVB2 | 24041 | 35114 | 1.76% | 0.135% |
| 3 | 5.010 | 494 | 497 | 511 | rVB | 164971 | 209399 | 10.48% | 0.806% |
| 4 | 5.398 | 559 | 563 | 567 | rBV2 | 36979 | 53113 | 2.66% | 0.205% |
| 5 | 5.439 | 567 | 570 | 591 | rVB | 1217873 | 1400777 | 70.12% | 5.395% |
| 6 | 5.722 | 615 | 618 | 625 | rVB | 41249 | 37422 | 1.87% | 0.144% |
| 7 | 6.339 | 720 | 723 | 726 | rBV2 | 33432 | 29748 | 1.49% | 0.115% |
| 8 | 6.457 | 740 | 743 | 758 | rBV | 1637105 | 1707765 | 85.49% | 6.577% |
| 9 | 6.586 | 761 | 765 | 771 | rVV | 1838347 | 1632779 | 81.74% | 6.288% |
| 10 | 6.645 | 771 | 775 | 780 | rVB2 | 68369 | 93231 | 4.67% | 0.359% |
| 11 | 6.810 | 800 | 803 | 811 | rBV | 1077077 | 941489 | 47.13% | 3.626% |
| 12 | 6.869 | 811 | 813 | 818 | rBV3 | 23528 | 28781 | 1.44% | 0.111% |
| 13 | 6.969 | 826 | 830 | 841 | rVB | 1475691 | 1324004 | 66.28% | 5.099% |
| 14 | 7.086 | 847 | 850 | 853 | rVB | 27369 | 23951 | 1.20% | 0.092% |
| 15 | 7.204 | 864 | 870 | 873 | rBV2 | 20266 | 24785 | 1.24% | 0.095% |
| 16 | 7.345 | 889 | 894 | 896 | rBV2 | 27693 | 30252 | 1.51% | 0.117% |
| 17 | 7.375 | 896 | 899 | 903 | rVV | 1133961 | 1022096 | 51.17% | 3.936% |
| 18 | 7.404 | 903 | 904 | 910 | rVV | 83428 | 83821 | 4.20% | 0.323% |
| 19 | 7.457 | 910 | 913 | 916 | rVB4 | 21623 | 24660 | 1.23% | 0.095% |
| 20 | 7.910 | 984 | 990 | 997 | rVB7 | 14329 | 29945 | 1.50% | 0.115% |
| 21 | 7.963 | 997 | 999 | 1003 | rBV2 | 13977 | 23405 | 1.17% | 0.090% |
| 22 | 8.092 | 1015 | 1021 | 1029 | rBV | 1513275 | 1374304 | 68.80% | 5.293% |
| 23 | 8.386 | 1063 | 1071 | 1075 | rBV6 | 25136 | 44873 | 2.25% | 0.173% |
| 24 | 8.516 | 1089 | 1093 | 1095 | rBV | 32669 | 31900 | 1.60% | 0.123% |
| 25 | 8.686 | 1118 | 1122 | 1124 | rBV | 43345 | 41782 | 2.09% | 0.161% |
| 26 | 8.810 | 1141 | 1143 | 1146 | rBV | 51948 | 42181 | 2.11% | 0.162% |
| 27 | 8.910 | 1156 | 1160 | 1167 | rVB | 30456 | 42139 | 2.11% | 0.162% |
| 28 | 9.110 | 1192 | 1194 | 1200 | rBV | 36528 | 38109 | 1.91% | 0.147% |
| 29 | 9.169 | 1200 | 1204 | 1207 | rBV | 2399288 | 1997546 | 100.00% | 7.693% |
| 30 | 9.245 | 1214 | 1217 | 1220 | rBV | 56777 | 55582 | 2.78% | 0.214% |
| 31 | 9.439 | 1246 | 1250 | 1253 | rBV2 | 28025 | 32736 | 1.64% | 0.126% |
| 32 | 9.510 | 1258 | 1262 | 1264 | rVV | 32688 | 37288 | 1.87% | 0.144% |
| 33 | 9.563 | 1268 | 1271 | 1279 | rVB | 312148 | 284575 | 14.25% | 1.096% |
| 34 | 9.710 | 1293 | 1296 | 1299 | rBV | 81995 | 81136 | 4.06% | 0.312% |

LSC Area Percent Report

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Data File : BF114552.D
Acq On : 24 May 2019 4:12
Operator : JU/SJ
Sample : K3008-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-21

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-BF051019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 9.774 | 1305 | 1307 | 1312 | rVB | 43627 | 40677 | 2.04% | 0.157% |
| 36 | 9.851 | 1316 | 1320 | 1323 | rVV | 1554078 | 1438991 | 72.04% | 5.542% |
| 37 | 9.880 | 1323 | 1325 | 1330 | rVB2 | 48260 | 45422 | 2.27% | 0.175% |
| 38 | 9.951 | 1335 | 1337 | 1341 | rVB4 | 22948 | 27960 | 1.40% | 0.108% |
| 39 | 10.057 | 1352 | 1355 | 1359 | rVB2 | 42272 | 44575 | 2.23% | 0.172% |
| 40 | 10.092 | 1359 | 1361 | 1366 | rVB3 | 25373 | 24954 | 1.25% | 0.096% |
| 41 | 10.163 | 1370 | 1373 | 1377 | rBV4 | 25928 | 35997 | 1.80% | 0.139% |
| 42 | 10.251 | 1385 | 1388 | 1390 | rBV2 | 33494 | 33927 | 1.70% | 0.131% |
| 43 | 10.274 | 1390 | 1392 | 1395 | rVB | 57082 | 43131 | 2.16% | 0.166% |
| 44 | 10.398 | 1410 | 1413 | 1418 | rVB2 | 42167 | 51422 | 2.57% | 0.198% |
| 45 | 10.492 | 1426 | 1429 | 1436 | rVB4 | 26770 | 40949 | 2.05% | 0.158% |
| 46 | 10.639 | 1450 | 1454 | 1464 | rVB | 960921 | 905960 | 45.35% | 3.489% |
| 47 | 10.745 | 1470 | 1472 | 1473 | rBV | 56594 | 41955 | 2.10% | 0.162% |
| 48 | 10.945 | 1503 | 1506 | 1509 | rBV5 | 19008 | 24827 | 1.24% | 0.096% |
| 49 | 11.145 | 1537 | 1540 | 1544 | rBV | 52717 | 56315 | 2.82% | 0.217% |
| 50 | 11.192 | 1544 | 1548 | 1550 | rVV2 | 73360 | 76465 | 3.83% | 0.294% |
| 51 | 11.227 | 1551 | 1554 | 1560 | rVB3 | 59061 | 86148 | 4.31% | 0.332% |
| 52 | 11.333 | 1569 | 1572 | 1575 | rBV | 1602181 | 1537623 | 76.98% | 5.922% |
| 53 | 11.357 | 1575 | 1576 | 1580 | rVV | 675695 | 540325 | 27.05% | 2.081% |
| 54 | 11.410 | 1583 | 1585 | 1589 | rVB | 110826 | 104778 | 5.25% | 0.404% |
| 55 | 11.574 | 1609 | 1613 | 1617 | rBV2 | 85472 | 113708 | 5.69% | 0.438% |
| 56 | 11.621 | 1618 | 1621 | 1625 | rVB3 | 55515 | 52077 | 2.61% | 0.201% |
| 57 | 11.839 | 1655 | 1658 | 1660 | rBV | 109914 | 104093 | 5.21% | 0.401% |
| 58 | 11.868 | 1660 | 1663 | 1668 | rVV2 | 161816 | 203635 | 10.19% | 0.784% |
| 59 | 11.916 | 1669 | 1671 | 1674 | rVV | 50837 | 44269 | 2.22% | 0.170% |
| 60 | 11.951 | 1674 | 1677 | 1679 | rVV | 132228 | 143833 | 7.20% | 0.554% |
| 61 | 11.974 | 1679 | 1681 | 1684 | rVB | 77708 | 63527 | 3.18% | 0.245% |
| 62 | 12.027 | 1687 | 1690 | 1692 | rBV2 | 57838 | 54008 | 2.70% | 0.208% |
| 63 | 12.127 | 1705 | 1707 | 1711 | rBV | 71109 | 74302 | 3.72% | 0.286% |
| 64 | 12.168 | 1712 | 1714 | 1718 | rVB | 64660 | 61826 | 3.10% | 0.238% |
| 65 | 12.316 | 1736 | 1739 | 1741 | rVB2 | 35490 | 31703 | 1.59% | 0.122% |
| 66 | 12.386 | 1749 | 1751 | 1754 | rBV | 61786 | 57579 | 2.88% | 0.222% |
| 67 | 12.416 | 1754 | 1756 | 1759 | rBV3 | 58951 | 59251 | 2.97% | 0.228% |
| 68 | 12.480 | 1765 | 1767 | 1771 | rVB2 | 59615 | 57223 | 2.86% | 0.220% |
| 69 | 12.551 | 1775 | 1779 | 1783 | rBV | 986850 | 833451 | 41.72% | 3.210% |
| 70 | 12.645 | 1793 | 1795 | 1800 | rBV3 | 43549 | 46728 | 2.34% | 0.180% |
| 71 | 12.780 | 1812 | 1818 | 1824 | rBV | 854584 | 894535 | 44.78% | 3.445% |

LSC Area Percent Report

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Data File : BF114552.D
Acq On : 24 May 2019 4:12
Operator : JU/SJ
Sample : K3008-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-21

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-BF051019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 72 | 12.915 | 1837 | 1841 | 1844 | rBV | 1969535 | 1642457 | 82.22% | 6.326% |
| 73 | 13.815 | 1991 | 1994 | 1996 | rBV | 132410 | 166410 | 8.33% | 0.641% |
| 74 | 13.980 | 2018 | 2022 | 2025 | rBV2 | 1191220 | 1390868 | 69.63% | 5.357% |
| 75 | 14.004 | 2025 | 2026 | 2030 | rVB | 333593 | 266174 | 13.33% | 1.025% |
| 76 | 15.021 | 2196 | 2199 | 2202 | rBV | 244891 | 319589 | 16.00% | 1.231% |
| 77 | 15.386 | 2258 | 2261 | 2265 | rVB | 227276 | 283543 | 14.19% | 1.092% |
| 78 | 15.445 | 2267 | 2271 | 2275 | rVB | 676040 | 887839 | 44.45% | 3.419% |

Sum of corrected areas: 25964980

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052319\
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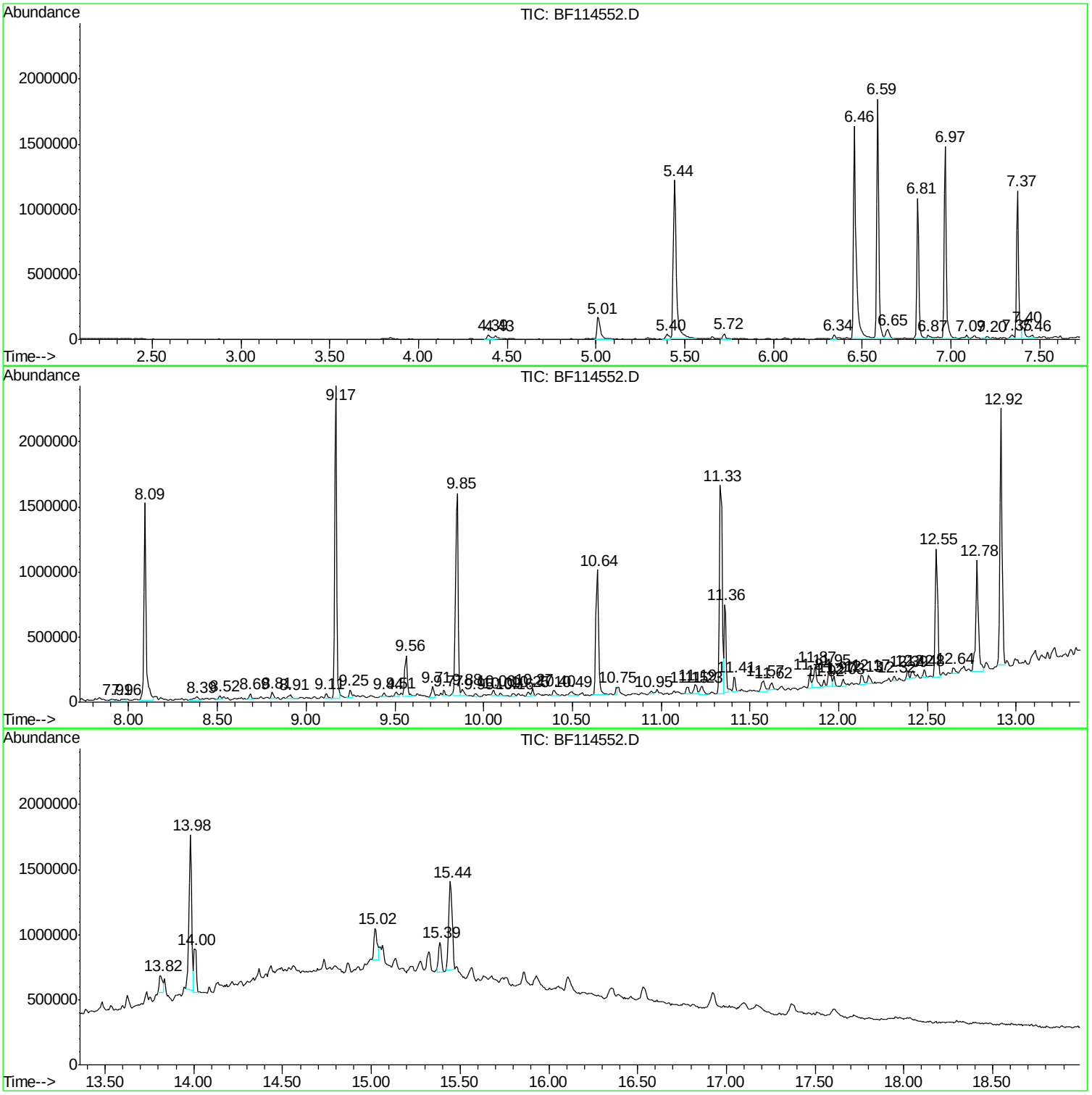
Sample : K3008-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
COMP-21

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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\BF052319\
Data File : BF114552.D
Acq On : 24 May 2019 4:12
Operator : JU/SJ
Sample : K3008-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-21

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

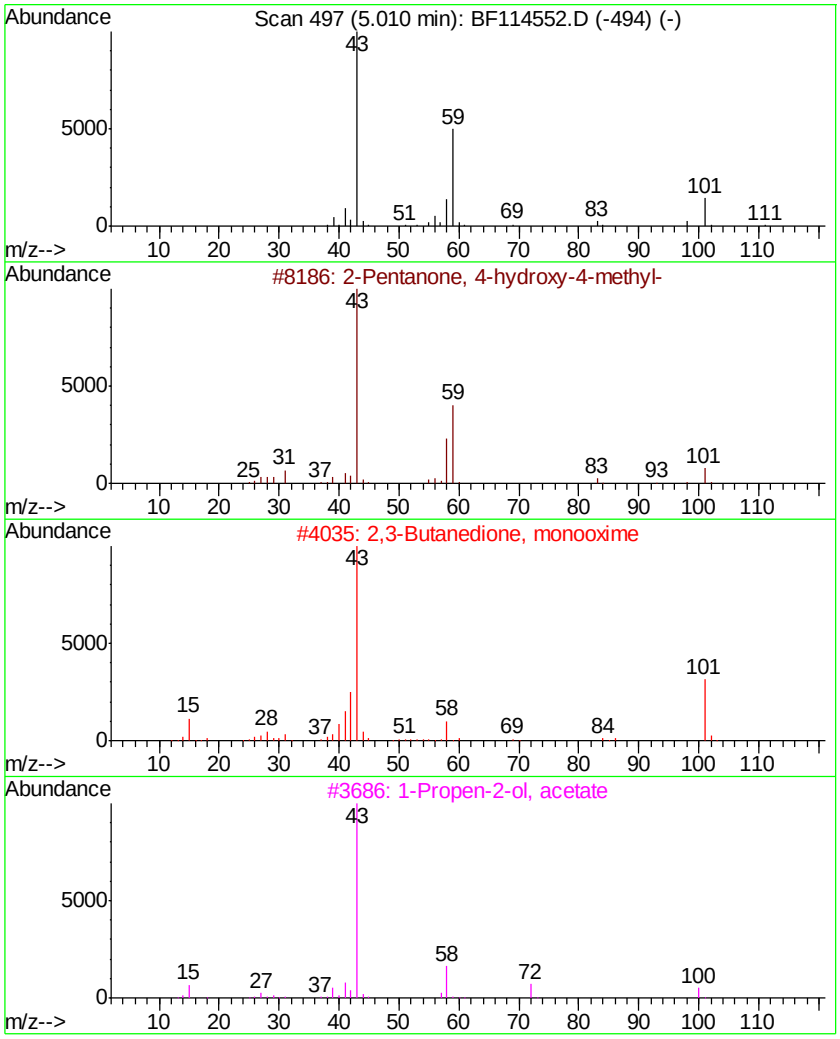
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

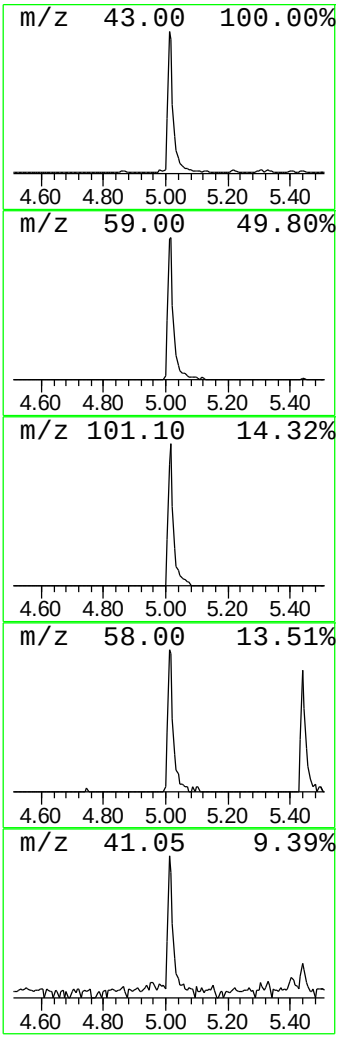
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.01 | 4.45 ng | 209399 | 1,4-Dichlorobenzene-d4 | 6.81 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 3 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 9 |
| 4 | Formamide, N,N-diethyl- | 101 | C5H11NO | 000617-84-5 | 7 |
| 5 | Butane | 58 | C4H10 | 000106-97-8 | 5 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052319\
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Operator : JU/SJ
Sample : K3008-05
Misc :
ALS Vial : 21 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-21

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

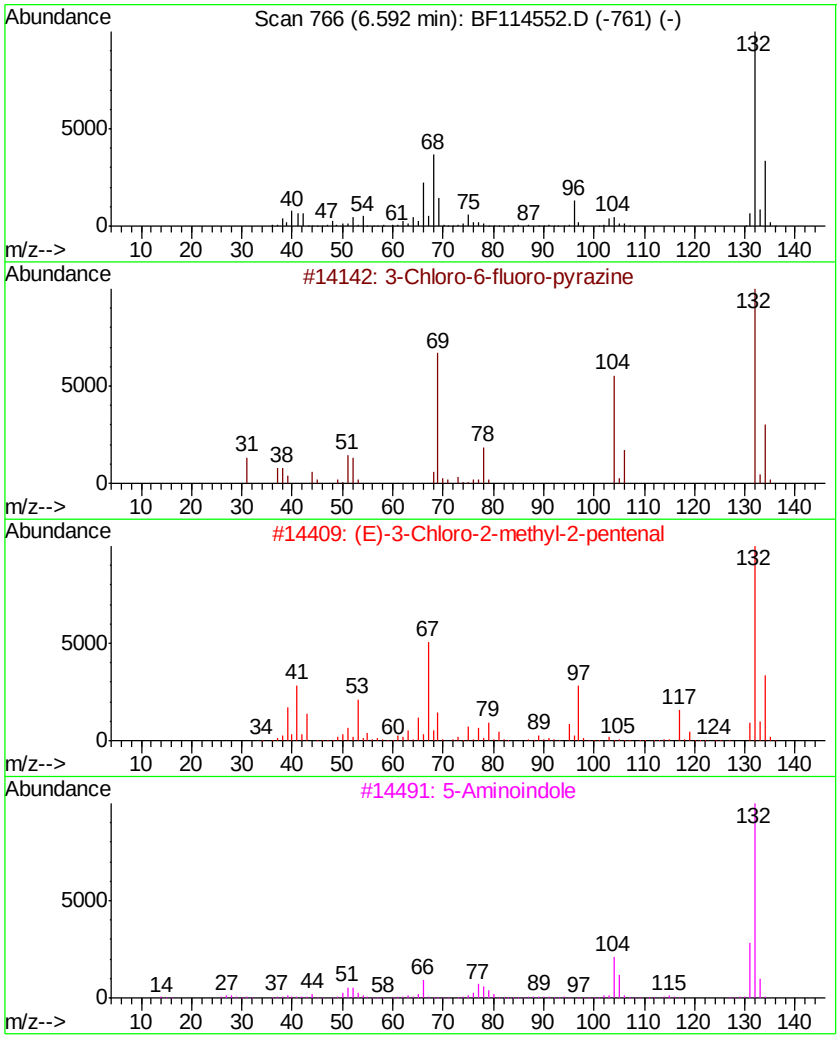
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

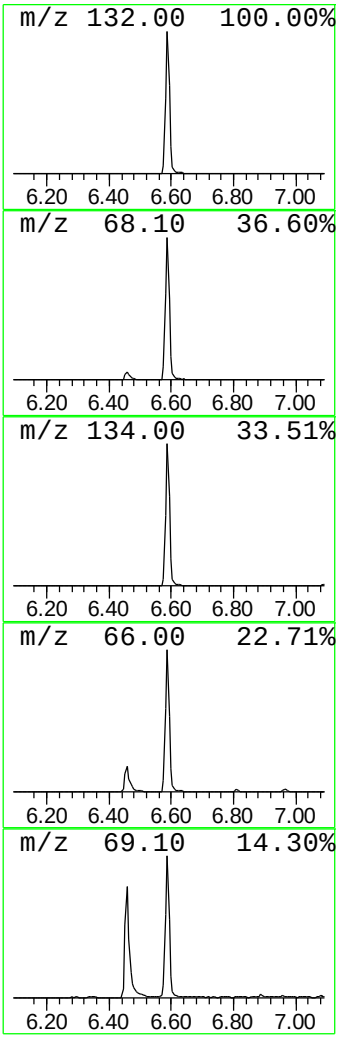
**********

Peak Number 2 unknown6.59 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.59 | 34.69 ng | 1632780 | 1,4-Dichlorobenzene-d4 | 6.81 |

| 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 | 17 |
| 3 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 4 | Amphetaminil | 250 | C17H18N2 | 017590-01-1 | 10 |
| 5 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |



# Library Search Compound Report

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Misc :
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**Instrument :** BNA_F
**ClientSampleId :** COMP-21

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

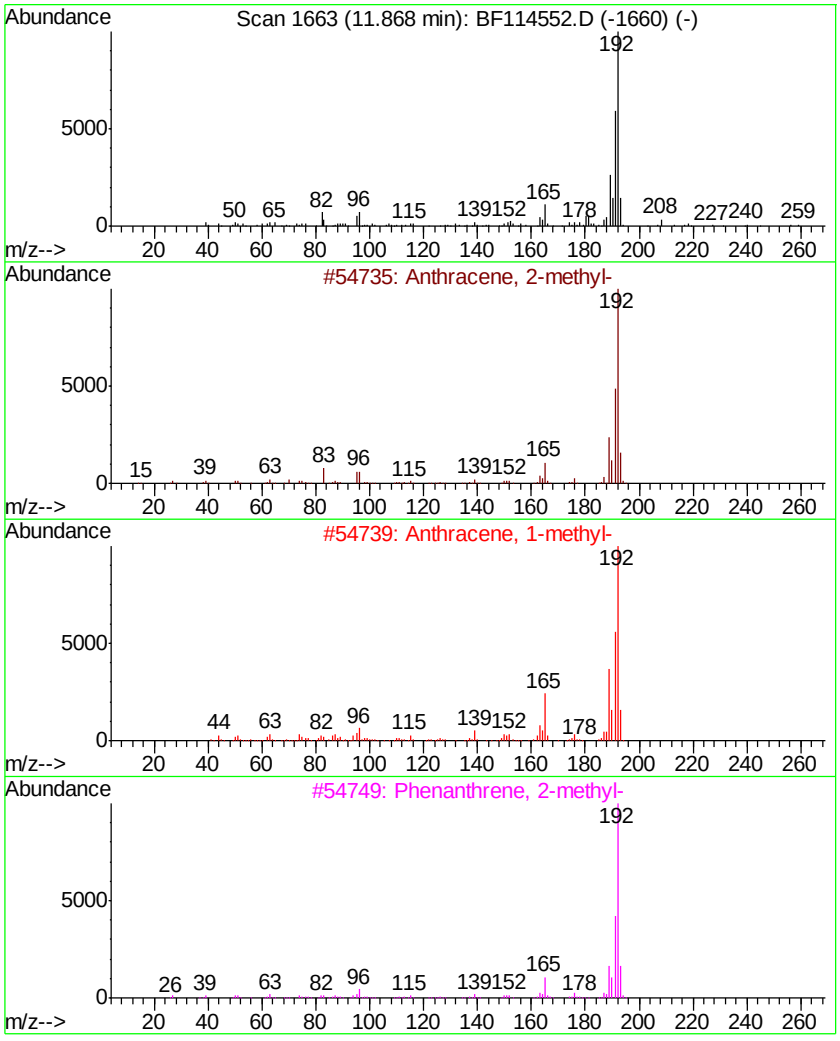
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

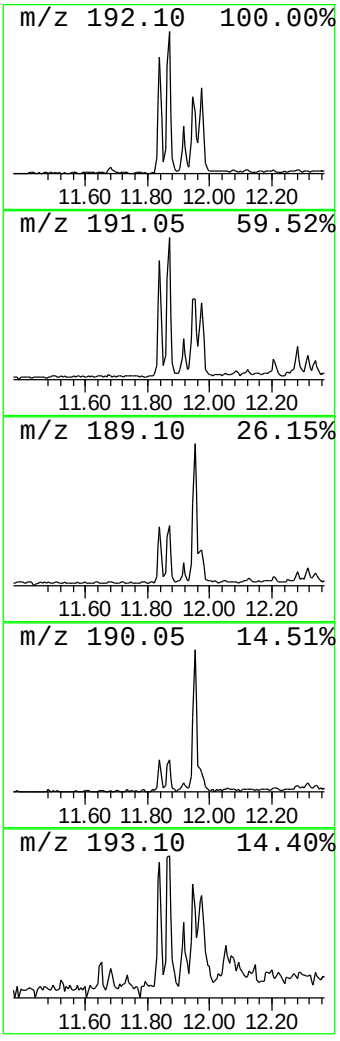
**********

Peak Number 4 Anthracene, 2-methyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.87 | 2.65 ng | 203635 | Phenanthrene-d10 | 11.33 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Anthracene, 2-methyl- | 192 | C15H12 | 000613-12-7 | 96 |
| 2 | Anthracene, 1-methyl- | 192 | C15H12 | 000610-48-0 | 94 |
| 3 | Phenanthrene, 2-methyl- | 192 | C15H12 | 002531-84-2 | 93 |
| 4 | Anthracene, 9-methyl- | 192 | C15H12 | 000779-02-2 | 93 |
| 5 | 1H-Cyclopropa[l]phenanthrene,1a,... | 192 | C15H12 | 000949-41-7 | 89 |



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

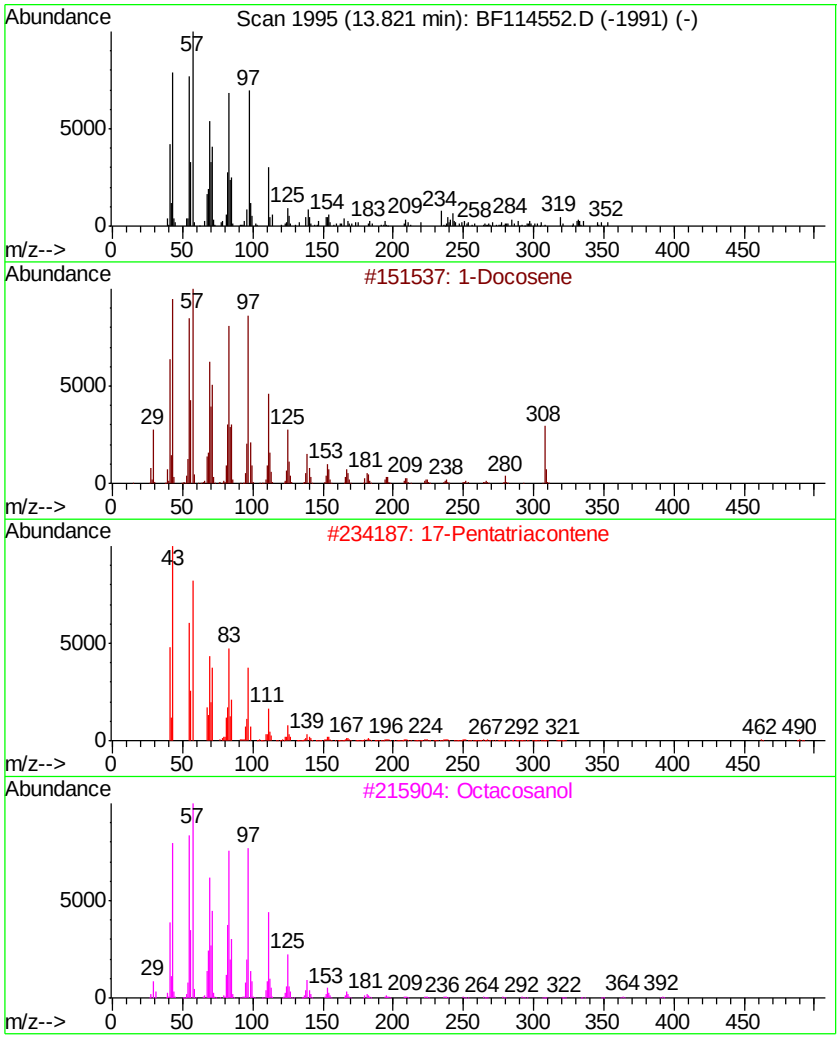
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

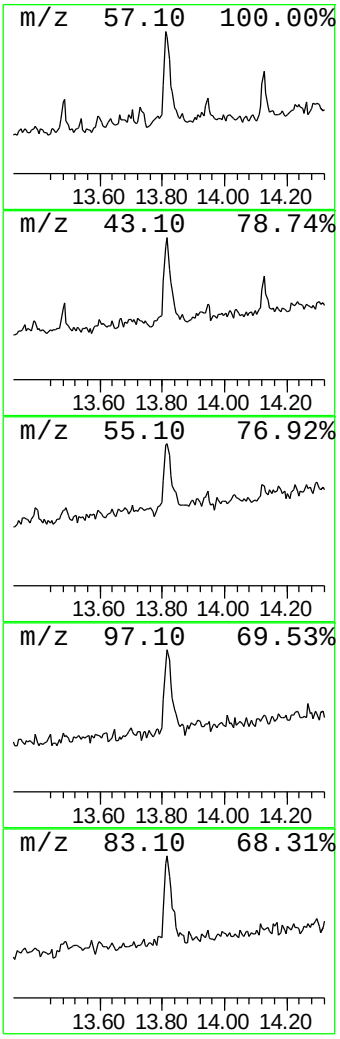
**********

Peak Number 5 1-Docosene Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.82 | 2.39 ng | 166410 | Chrysene-d12 | 13.98 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 93 |
| 2 | 17-Pentatriacontene | 491 | C35H70 | 006971-40-0 | 90 |
| 3 | Octacosanol | 410 | C28H58O | 000557-61-9 | 83 |
| 4 | Ethanol, 2-(tetradecyloxy)- | 258 | C16H34O2 | 002136-70-1 | 83 |
| 5 | 1-Hexadecanesulfonyl chloride | 324 | C16H33ClO2S | 038775-38-1 | 83 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF052319\
Data File : BF114552.D
Acq On : 24 May 2019 4:12
Operator : JU/SJ
Sample : K3008-05
Misc :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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 |
| 2-Pentanone, 4-hy... | 5.01 | 4.5 | ng | 209399 | 1 | 6.81 | 941489 | 20.0 |
| unknown6.59 | 6.59 | 34.7 | ng | 1632780 | 1 | 6.81 | 941489 | 20.0 |
| Anthracene, 2-met... | 11.87 | 2.6 | ng | 203635 | 4 | 11.33 | 1537620 | 20.0 |
| 1-Docosene | 13.82 | 2.4 | ng | 166410 | 5 | 13.98 | 1390870 | 20.0 |