LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091417\
Data File : BF098552.D
Acq On : 15 Sep 2017 2:36
Operator : SJ/JU
Sample : I5222-05 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SP-2

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:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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 | 4.810 | 460 | 463 | 476 | rBV | 152218 | 185019 | 9.96% | 0.843% |
| 2 | 5.251 | 534 | 538 | 554 | rBV | 1522966 | 1751081 | 94.24% | 7.977% |
| 3 | 6.304 | 713 | 717 | 734 | rBV | 1542307 | 1858122 | 100.00% | 8.464% |
| 4 | 6.422 | 734 | 737 | 743 | rVB | 2014912 | 1788772 | 96.27% | 8.148% |
| 5 | 6.645 | 771 | 775 | 781 | rBV | 994797 | 817098 | 43.97% | 3.722% |
| 6 | 6.798 | 798 | 801 | 812 | rBV | 1317952 | 1281018 | 68.94% | 5.835% |
| 7 | 7.216 | 868 | 872 | 884 | rBV | 1206870 | 1084419 | 58.36% | 4.940% |
| 8 | 7.927 | 990 | 993 | 996 | rBV | 1174952 | 1092852 | 58.81% | 4.978% |
| 9 | 8.645 | 1113 | 1115 | 1118 | rVB | 34564 | 25151 | 1.35% | 0.115% |
| 10 | 8.745 | 1127 | 1132 | 1135 | rBV | 27129 | 30831 | 1.66% | 0.140% |
| 11 | 9.004 | 1172 | 1176 | 1180 | rBV | 2186269 | 1828973 | 98.43% | 8.331% |
| 12 | 9.274 | 1218 | 1222 | 1225 | rBV2 | 20151 | 25256 | 1.36% | 0.115% |
| 13 | 9.345 | 1230 | 1234 | 1236 | rBV | 35486 | 38167 | 2.05% | 0.174% |
| 14 | 9.404 | 1241 | 1244 | 1247 | rVV | 304167 | 242111 | 13.03% | 1.103% |
| 15 | 9.457 | 1251 | 1253 | 1258 | rVB4 | 17297 | 22124 | 1.19% | 0.101% |
| 16 | 9.545 | 1265 | 1268 | 1273 | rBV | 35429 | 42983 | 2.31% | 0.196% |
| 17 | 9.586 | 1273 | 1275 | 1278 | rVB4 | 26980 | 22631 | 1.22% | 0.103% |
| 18 | 9.616 | 1278 | 1280 | 1284 | rBV | 31223 | 31458 | 1.69% | 0.143% |
| 19 | 9.680 | 1284 | 1291 | 1294 | rBV2 | 1424227 | 1194987 | 64.31% | 5.443% |
| 20 | 9.710 | 1294 | 1296 | 1300 | rVB | 103597 | 90853 | 4.89% | 0.414% |
| 21 | 9.886 | 1320 | 1326 | 1330 | rBV | 71083 | 68606 | 3.69% | 0.313% |
| 22 | 9.927 | 1330 | 1333 | 1337 | rVB3 | 16095 | 23102 | 1.24% | 0.105% |
| 23 | 9.998 | 1342 | 1345 | 1348 | rBV3 | 18160 | 22171 | 1.19% | 0.101% |
| 24 | 10.086 | 1356 | 1360 | 1362 | rBV4 | 28769 | 30519 | 1.64% | 0.139% |
| 25 | 10.116 | 1362 | 1365 | 1367 | rVV | 43557 | 35526 | 1.91% | 0.162% |
| 26 | 10.227 | 1381 | 1384 | 1387 | rBV2 | 94949 | 87845 | 4.73% | 0.400% |
| 27 | 10.333 | 1400 | 1402 | 1405 | rVB2 | 32450 | 25686 | 1.38% | 0.117% |
| 28 | 10.386 | 1408 | 1411 | 1415 | rVB2 | 31008 | 36576 | 1.97% | 0.167% |
| 29 | 10.469 | 1419 | 1425 | 1430 | rBV | 1087535 | 983334 | 52.92% | 4.479% |
| 30 | 10.598 | 1442 | 1447 | 1450 | rBV2 | 75629 | 114316 | 6.15% | 0.521% |
| 31 | 10.657 | 1453 | 1457 | 1460 | rBV5 | 14386 | 22298 | 1.20% | 0.102% |
| 32 | 11.033 | 1519 | 1521 | 1523 | rBV | 43883 | 34573 | 1.86% | 0.157% |
| 33 | 11.063 | 1523 | 1526 | 1531 | rVB | 66627 | 72873 | 3.92% | 0.332% |
| 34 | 11.163 | 1539 | 1543 | 1545 | rBV | 1235714 | 1057986 | 56.94% | 4.819% |

LSC Area Percent Report

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Operator : SJ/JU
Sample : I5222-05 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SP-2

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:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 11.186 | 1545 | 1547 | 1550 | rVV | 391129 | 309949 | 16.68% | 1.412% |
| 36 | 11.239 | 1553 | 1556 | 1559 | rVB | 72462 | 65703 | 3.54% | 0.299% |
| 37 | 11.404 | 1580 | 1584 | 1588 | rBV2 | 23379 | 35659 | 1.92% | 0.162% |
| 38 | 11.457 | 1591 | 1593 | 1596 | rVB2 | 39384 | 28977 | 1.56% | 0.132% |
| 39 | 11.663 | 1625 | 1628 | 1631 | rBV | 46646 | 45575 | 2.45% | 0.208% |
| 40 | 11.692 | 1631 | 1633 | 1636 | rVB | 59348 | 51516 | 2.77% | 0.235% |
| 41 | 11.739 | 1637 | 1641 | 1644 | rBV3 | 22508 | 32581 | 1.75% | 0.148% |
| 42 | 11.774 | 1644 | 1647 | 1649 | rVV | 106399 | 104786 | 5.64% | 0.477% |
| 43 | 11.798 | 1649 | 1651 | 1656 | rVB | 40271 | 35214 | 1.90% | 0.160% |
| 44 | 11.957 | 1675 | 1678 | 1680 | rBV2 | 36533 | 31012 | 1.67% | 0.141% |
| 45 | 11.992 | 1682 | 1684 | 1688 | rVB5 | 24626 | 23977 | 1.29% | 0.109% |
| 46 | 12.210 | 1718 | 1721 | 1724 | rBV2 | 43667 | 40172 | 2.16% | 0.183% |
| 47 | 12.251 | 1725 | 1728 | 1733 | rVB3 | 43697 | 56585 | 3.05% | 0.258% |
| 48 | 12.304 | 1733 | 1737 | 1740 | rBV3 | 27427 | 33787 | 1.82% | 0.154% |
| 49 | 12.368 | 1745 | 1748 | 1752 | rBV | 410678 | 377494 | 20.32% | 1.720% |
| 50 | 12.598 | 1781 | 1787 | 1790 | rBV | 395060 | 386169 | 20.78% | 1.759% |
| 51 | 12.621 | 1790 | 1791 | 1794 | rVB | 39734 | 22989 | 1.24% | 0.105% |
| 52 | 12.651 | 1794 | 1796 | 1799 | rBV4 | 17776 | 21629 | 1.16% | 0.099% |
| 53 | 12.745 | 1808 | 1812 | 1815 | rBV | 1524374 | 1349832 | 72.64% | 6.149% |
| 54 | 12.821 | 1821 | 1825 | 1828 | rBV4 | 30262 | 42791 | 2.30% | 0.195% |
| 55 | 12.927 | 1837 | 1843 | 1846 | rVB | 55848 | 71121 | 3.83% | 0.324% |
| 56 | 12.992 | 1853 | 1854 | 1857 | rVB2 | 39287 | 24420 | 1.31% | 0.111% |
| 57 | 13.027 | 1857 | 1860 | 1863 | rBV3 | 41531 | 52158 | 2.81% | 0.238% |
| 58 | 13.151 | 1879 | 1881 | 1884 | rBV | 22639 | 23405 | 1.26% | 0.107% |
| 59 | 13.439 | 1928 | 1930 | 1933 | rVB | 39874 | 34044 | 1.83% | 0.155% |
| 60 | 13.545 | 1945 | 1948 | 1950 | rBV | 30580 | 29321 | 1.58% | 0.134% |
| 61 | 13.645 | 1962 | 1965 | 1969 | rVB2 | 80758 | 84659 | 4.56% | 0.386% |
| 62 | 13.792 | 1985 | 1990 | 1993 | rBV2 | 930034 | 1089232 | 58.62% | 4.962% |
| 63 | 13.821 | 1993 | 1995 | 1998 | rVB | 122723 | 102126 | 5.50% | 0.465% |
| 64 | 14.804 | 2158 | 2162 | 2169 | rBV | 125958 | 208933 | 11.24% | 0.952% |
| 65 | 15.080 | 2206 | 2209 | 2215 | rVB | 76925 | 81001 | 4.36% | 0.369% |
| 66 | 15.133 | 2215 | 2218 | 2223 | rVB | 108476 | 126242 | 6.79% | 0.575% |
| 67 | 15.192 | 2224 | 2228 | 2235 | rBV | 713745 | 860376 | 46.30% | 3.919% |

Sum of corrected areas: 21952752

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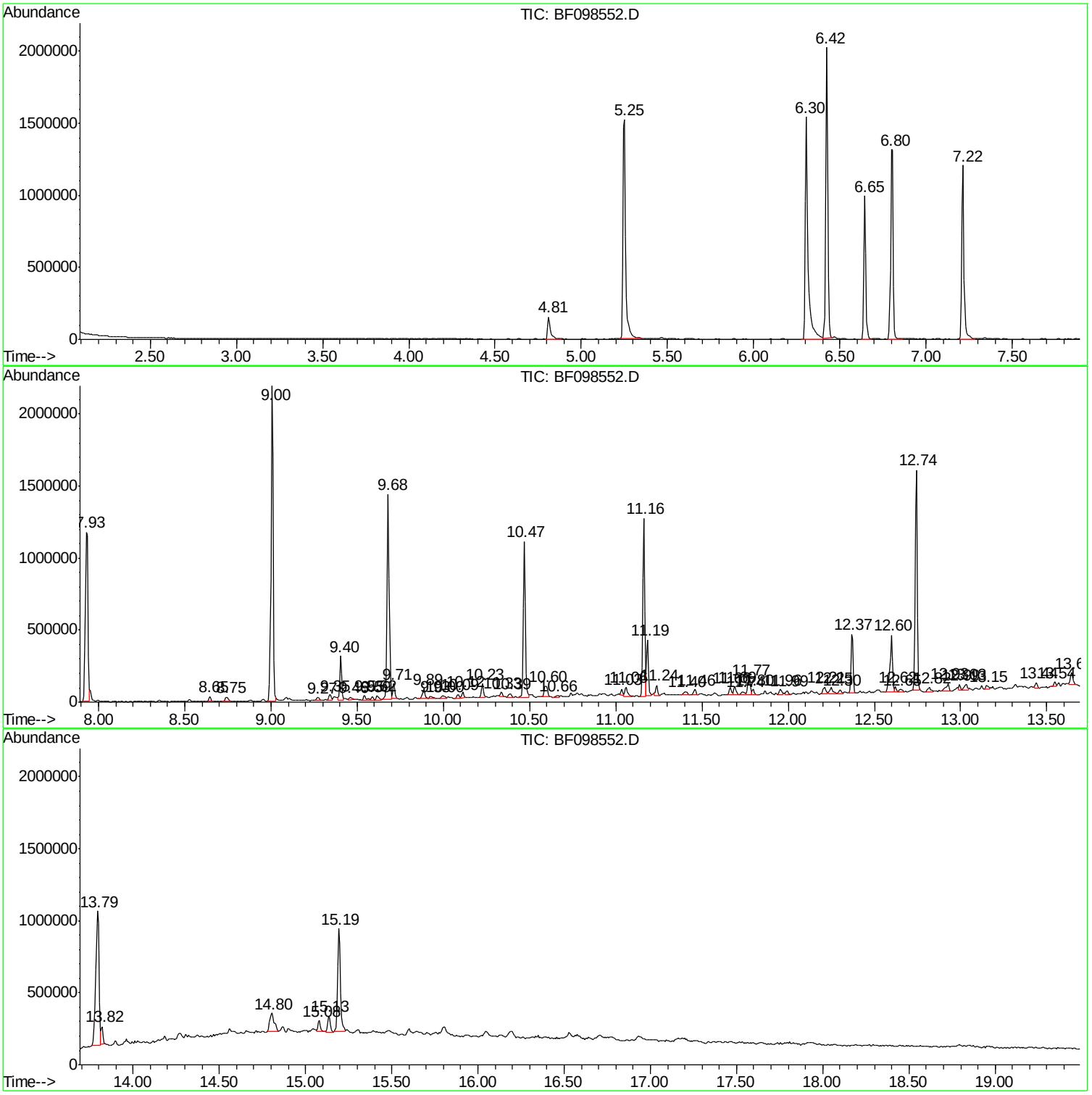
Sample : I5222-05 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
SP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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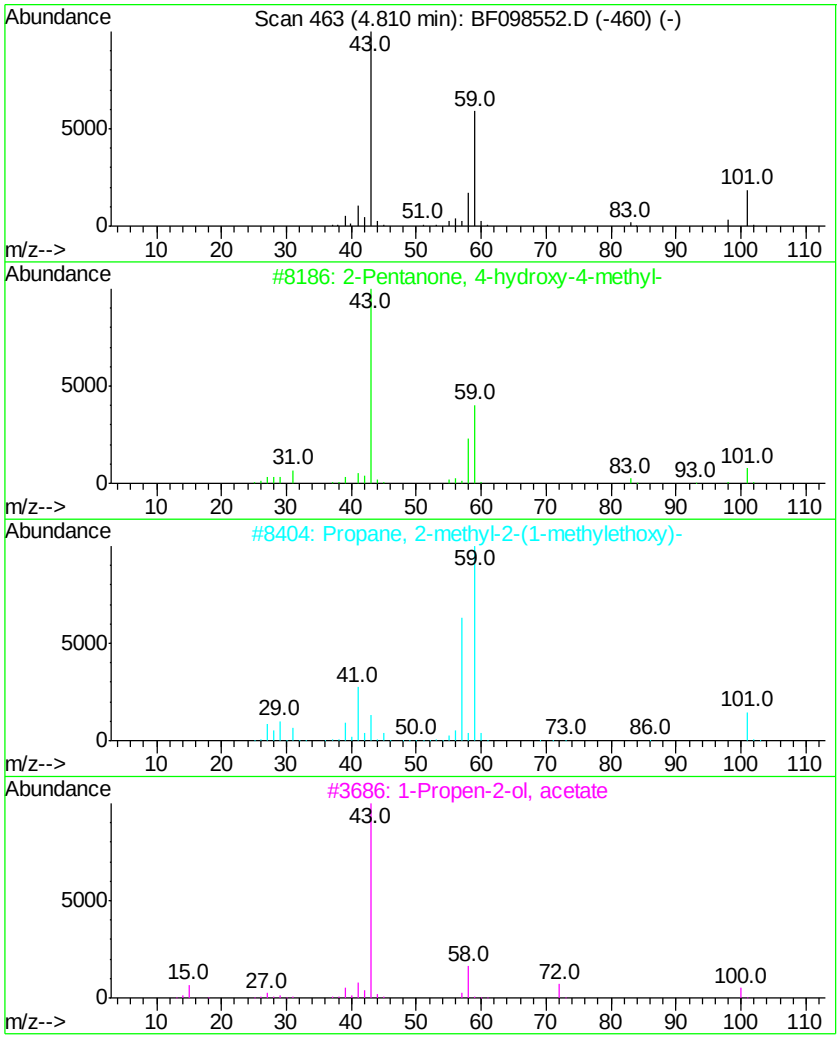
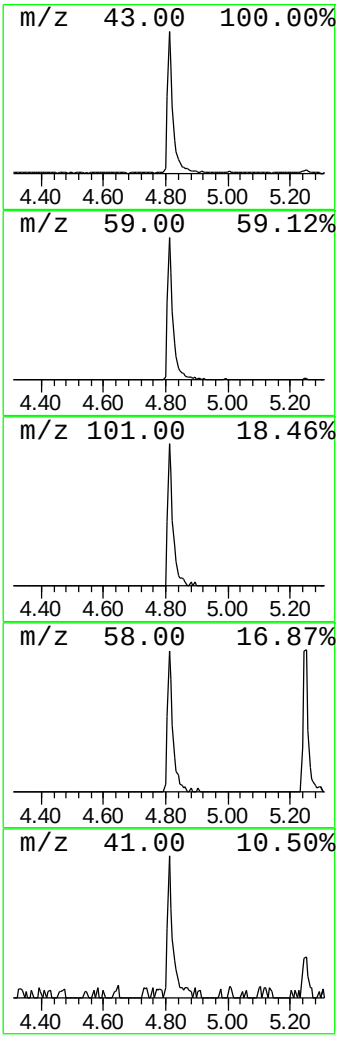
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.81 | 4.53 ng | 185019 | 1,4-Dichlorobenzene-d4 | 6.65 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 42 |
| 3 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 10 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 5 | Propane, 1-ethoxy-2-methyl- | 102 | C6H14O | 000627-02-1 | 9 |



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ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

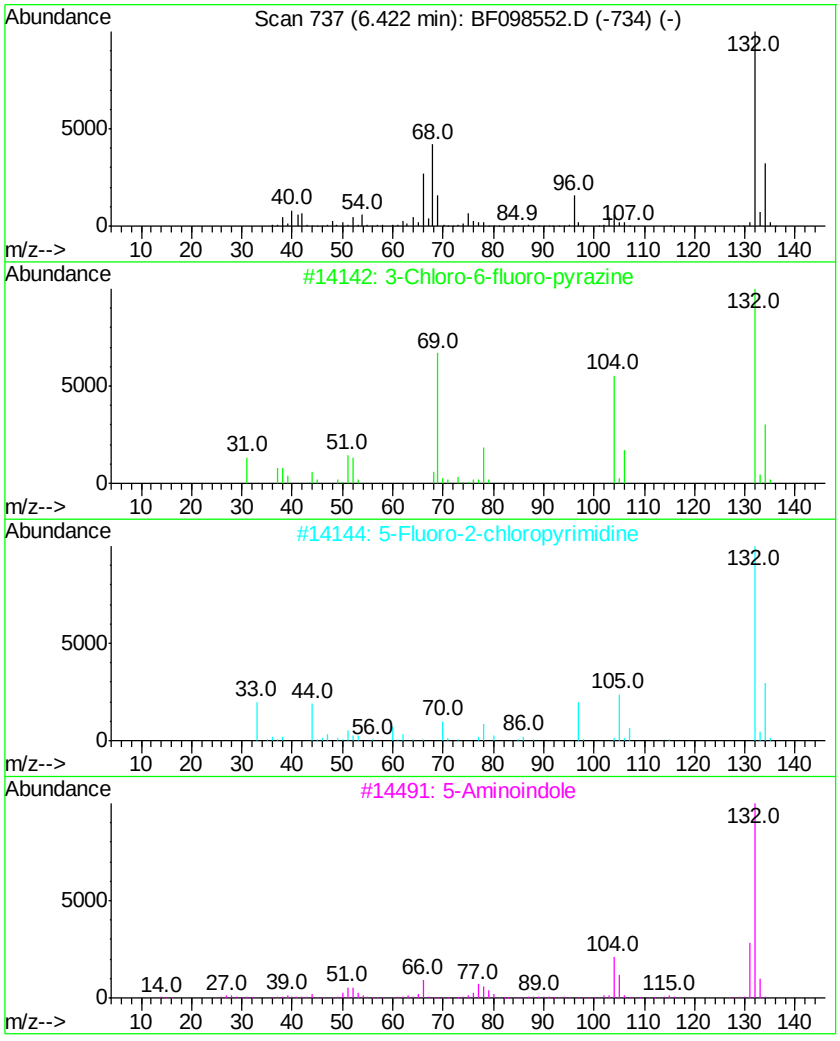
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

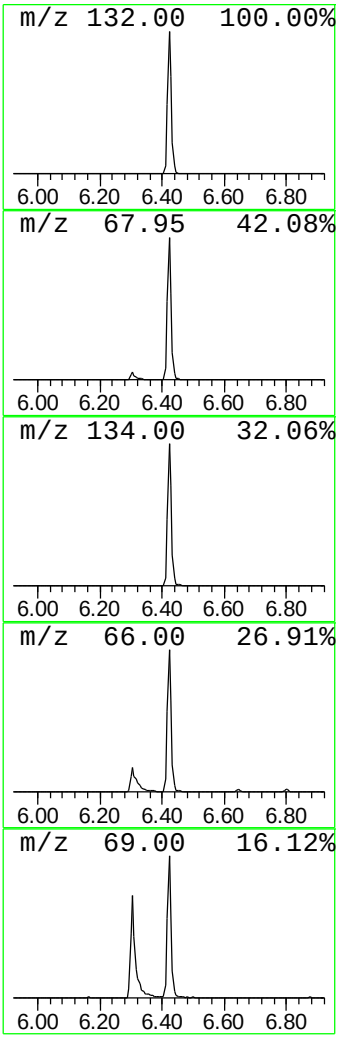
**********

Peak Number 2 unknown6.42 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.42 | 43.78 ng | 1788770 | 1,4-Dichlorobenzene-d4 | 6.65 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 12 |
| 3 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 4 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 5 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |



# Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091417\
Data File : BF098552.D
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Sample : I5222-05 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SP-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

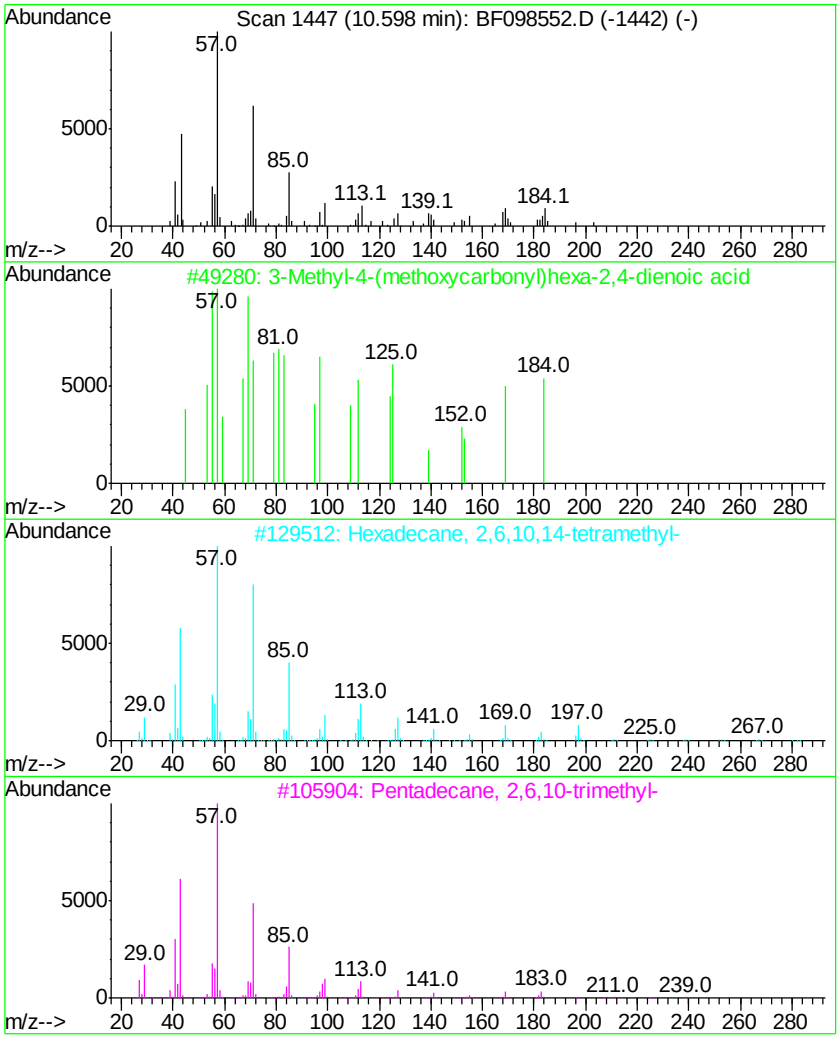
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

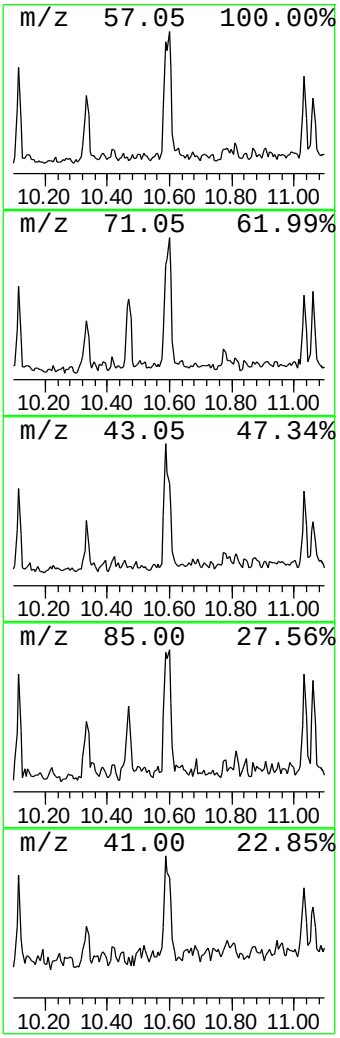
**********

Peak Number 4 3-Methyl-4-(methoxycarbonyl... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.60 | 2.16 ng | 114316 | Phenanthrene-d10 | 11.16 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Methyl-4-(methoxycarbonyl)hexa... | 184 | C9H12O4 | 1000104-10-8 | 86 |
| 2 | Hexadecane, 2,6,10,14-tetramethyl- | 282 | C20H42 | 000638-36-8 | 72 |
| 3 | Pentadecane, 2,6,10-trimethyl- | 254 | C18H38 | 003892-00-0 | 64 |
| 4 | Heptadecane | 240 | C17H36 | 000629-78-7 | 59 |
| 5 | Hexadecane, 2,6,11,15-tetramethyl- | 282 | C20H42 | 000504-44-9 | 58 |



Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 4.81 | 4.5 | ng | 185019 | 1 | 6.65 | 817098 | 20.0 |
| unknown6.42 | 6.42 | 43.8 | ng | 1788770 | 1 | 6.65 | 817098 | 20.0 |
| 3-Methyl-4-(metho... | 10.60 | 2.2 | ng | 114316 | 4 | 11.16 | 1057990 | 20.0 |