LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117337.D
Acq On : 4 Oct 2019 00:38
Operator : JU
Sample : K5140-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-05-100219

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-BF091319.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 | 5.398 | 556 | 563 | 567 | rBV2 | 45420 | 68660 | 5.65% | 0.281% |
| 2 | 5.440 | 567 | 570 | 578 | rVV | 231991 | 302268 | 24.88% | 1.239% |
| 3 | 5.716 | 614 | 617 | 624 | rVV | 123175 | 110587 | 9.10% | 0.453% |
| 4 | 5.963 | 653 | 659 | 664 | rVB3 | 54040 | 71122 | 5.85% | 0.291% |
| 5 | 6.057 | 672 | 675 | 681 | rVB3 | 129748 | 155662 | 12.81% | 0.638% |
| 6 | 6.245 | 702 | 707 | 710 | rBV2 | 88598 | 107238 | 8.83% | 0.439% |
| 7 | 6.310 | 716 | 718 | 720 | rVB | 104035 | 71797 | 5.91% | 0.294% |
| 8 | 6.340 | 720 | 723 | 725 | rBV2 | 272877 | 281167 | 23.14% | 1.152% |
| 9 | 6.363 | 725 | 727 | 730 | rVB | 90773 | 81884 | 6.74% | 0.336% |
| 10 | 6.410 | 730 | 735 | 740 | rVB2 | 147643 | 206391 | 16.99% | 0.846% |
| 11 | 6.457 | 740 | 743 | 746 | rBV | 291591 | 339293 | 27.92% | 1.390% |
| 12 | 6.492 | 748 | 749 | 755 | rVB2 | 116388 | 103398 | 8.51% | 0.424% |
| 13 | 6.551 | 755 | 759 | 762 | rBV | 95035 | 152436 | 12.55% | 0.625% |
| 14 | 6.587 | 762 | 765 | 770 | rVB | 424252 | 440848 | 36.28% | 1.806% |
| 15 | 6.645 | 770 | 775 | 781 | rVB2 | 696597 | 947194 | 77.96% | 3.881% |
| 16 | 6.751 | 786 | 793 | 794 | rBV4 | 57225 | 91610 | 7.54% | 0.375% |
| 17 | 6.810 | 799 | 803 | 810 | rVB3 | 298941 | 501568 | 41.28% | 2.055% |
| 18 | 6.869 | 810 | 813 | 817 | rVB | 233570 | 205811 | 16.94% | 0.843% |
| 19 | 6.963 | 825 | 829 | 832 | rBV2 | 417417 | 516662 | 42.52% | 2.117% |
| 20 | 6.992 | 832 | 834 | 836 | rVB | 114902 | 94090 | 7.74% | 0.386% |
| 21 | 7.087 | 847 | 850 | 852 | rVB | 362951 | 320575 | 26.38% | 1.314% |
| 22 | 7.128 | 852 | 857 | 859 | rBV2 | 282045 | 344466 | 28.35% | 1.411% |
| 23 | 7.151 | 859 | 861 | 866 | rVB3 | 217834 | 192558 | 15.85% | 0.789% |
| 24 | 7.198 | 866 | 869 | 873 | rBV2 | 416347 | 416836 | 34.31% | 1.708% |
| 25 | 7.234 | 873 | 875 | 879 | rVB4 | 59328 | 68212 | 5.61% | 0.279% |
| 26 | 7.275 | 879 | 882 | 884 | rBV | 123485 | 115732 | 9.53% | 0.474% |
| 27 | 7.298 | 884 | 886 | 889 | rVB | 129664 | 99078 | 8.15% | 0.406% |
| 28 | 7.345 | 889 | 894 | 896 | rBV | 317043 | 368633 | 30.34% | 1.510% |
| 29 | 7.369 | 896 | 898 | 902 | rVV3 | 208772 | 308398 | 25.38% | 1.264% |
| 30 | 7.410 | 902 | 905 | 908 | rVB | 1027420 | 807713 | 66.48% | 3.310% |
| 31 | 7.457 | 908 | 913 | 916 | rVB5 | 228677 | 335875 | 27.64% | 1.376% |
| 32 | 7.492 | 916 | 919 | 921 | rBV3 | 136814 | 178195 | 14.67% | 0.730% |
| 33 | 7.522 | 922 | 924 | 928 | rVB4 | 102887 | 93965 | 7.73% | 0.385% |
| 34 | 7.586 | 933 | 935 | 937 | rVV2 | 96525 | 115960 | 9.54% | 0.475% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117337.D
Acq On : 4 Oct 2019 00:38
Operator : JU
Sample : K5140-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-05-100219

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-BF091319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 7.616 | 937 | 940 | 943 | rVB3 | 301148 | 334034 | 27.49% | 1.369% |
| 36 | 7.692 | 949 | 953 | 954 | rBV2 | 125903 | 123568 | 10.17% | 0.506% |
| 37 | 7.710 | 954 | 956 | 958 | rVV2 | 162092 | 147675 | 12.15% | 0.605% |
| 38 | 7.734 | 958 | 960 | 963 | rVV4 | 144894 | 160993 | 13.25% | 0.660% |
| 39 | 7.775 | 963 | 967 | 970 | rVB3 | 260010 | 311960 | 25.68% | 1.278% |
| 40 | 7.810 | 970 | 973 | 974 | rBV | 294452 | 251335 | 20.69% | 1.030% |
| 41 | 7.839 | 974 | 978 | 983 | rVV5 | 300828 | 556955 | 45.84% | 2.282% |
| 42 | 7.886 | 983 | 986 | 988 | rVV2 | 185697 | 159196 | 13.10% | 0.652% |
| 43 | 7.910 | 988 | 990 | 991 | rVV | 131241 | 106906 | 8.80% | 0.438% |
| 44 | 7.928 | 991 | 993 | 996 | rVB | 233953 | 191984 | 15.80% | 0.787% |
| 45 | 7.957 | 996 | 998 | 1002 | rBV2 | 112632 | 122191 | 10.06% | 0.501% |
| 46 | 7.998 | 1002 | 1005 | 1008 | rBV | 90891 | 83748 | 6.89% | 0.343% |
| 47 | 8.051 | 1008 | 1014 | 1015 | rBV5 | 142788 | 228894 | 18.84% | 0.938% |
| 48 | 8.075 | 1015 | 1018 | 1023 | rVV3 | 980967 | 1183526 | 97.41% | 4.849% |
| 49 | 8.151 | 1027 | 1031 | 1034 | rVB2 | 391314 | 457582 | 37.66% | 1.875% |
| 50 | 8.181 | 1034 | 1036 | 1039 | rBV3 | 164295 | 152327 | 12.54% | 0.624% |
| 51 | 8.251 | 1044 | 1048 | 1049 | rBV4 | 77845 | 98978 | 8.15% | 0.406% |
| 52 | 8.286 | 1052 | 1054 | 1058 | rVB2 | 180620 | 186837 | 15.38% | 0.766% |
| 53 | 8.381 | 1065 | 1070 | 1077 | rBV5 | 314552 | 460086 | 37.87% | 1.885% |
| 54 | 8.439 | 1077 | 1080 | 1082 | rBV3 | 225387 | 209371 | 17.23% | 0.858% |
| 55 | 8.469 | 1082 | 1085 | 1088 | rBV3 | 255891 | 267982 | 22.06% | 1.098% |
| 56 | 8.510 | 1088 | 1092 | 1094 | rBV3 | 376651 | 338688 | 27.87% | 1.388% |
| 57 | 8.533 | 1094 | 1096 | 1098 | rVB | 108543 | 77764 | 6.40% | 0.319% |
| 58 | 8.557 | 1098 | 1100 | 1102 | rVB2 | 128655 | 103816 | 8.54% | 0.425% |
| 59 | 8.592 | 1103 | 1106 | 1109 | rBV2 | 342894 | 303554 | 24.98% | 1.244% |
| 60 | 8.633 | 1109 | 1113 | 1115 | rBV5 | 74200 | 79609 | 6.55% | 0.326% |
| 61 | 8.681 | 1118 | 1121 | 1125 | rBV | 772316 | 687903 | 56.62% | 2.819% |
| 62 | 8.722 | 1125 | 1128 | 1130 | rBV4 | 62381 | 77535 | 6.38% | 0.318% |
| 63 | 8.751 | 1130 | 1133 | 1134 | rVV3 | 102788 | 95379 | 7.85% | 0.391% |
| 64 | 8.775 | 1134 | 1137 | 1140 | rVB3 | 166404 | 226739 | 18.66% | 0.929% |
| 65 | 8.804 | 1140 | 1142 | 1145 | rVB3 | 99627 | 75418 | 6.21% | 0.309% |
| 66 | 8.839 | 1145 | 1148 | 1150 | rBV3 | 78650 | 68094 | 5.60% | 0.279% |
| 67 | 8.910 | 1158 | 1160 | 1166 | rVB4 | 188516 | 180657 | 14.87% | 0.740% |
| 68 | 8.963 | 1166 | 1169 | 1171 | rBV3 | 118051 | 118060 | 9.72% | 0.484% |
| 69 | 9.045 | 1179 | 1183 | 1187 | rVB2 | 164904 | 227681 | 18.74% | 0.933% |
| 70 | 9.081 | 1187 | 1189 | 1191 | rVV2 | 129793 | 105030 | 8.64% | 0.430% |
| 71 | 9.110 | 1191 | 1194 | 1200 | rVB3 | 272724 | 294118 | 24.21% | 1.205% |

LSC Area Percent Report

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Data File : BF117337.D
Acq On : 4 Oct 2019 00:38
Operator : JU
Sample : K5140-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-05-100219

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-BF091319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 72 | 9.163 | 1200 | 1203 | 1208 | rVB | 399863 | 348757 | 28.70% | 1.429% |
| 73 | 9.245 | 1213 | 1217 | 1220 | rBV | 487885 | 444762 | 36.60% | 1.822% |
| 74 | 9.286 | 1222 | 1224 | 1226 | rVV3 | 68141 | 76188 | 6.27% | 0.312% |
| 75 | 9.316 | 1226 | 1229 | 1232 | rVB2 | 137463 | 132848 | 10.93% | 0.544% |
| 76 | 9.498 | 1254 | 1260 | 1262 | rBV5 | 108929 | 155578 | 12.80% | 0.637% |
| 77 | 9.522 | 1262 | 1264 | 1266 | rVV3 | 84054 | 76581 | 6.30% | 0.314% |
| 78 | 9.563 | 1266 | 1271 | 1273 | rVV5 | 205181 | 268693 | 22.11% | 1.101% |
| 79 | 9.586 | 1273 | 1275 | 1278 | rVV2 | 110242 | 110350 | 9.08% | 0.452% |
| 80 | 9.622 | 1278 | 1281 | 1283 | rVB | 114209 | 86940 | 7.16% | 0.356% |
| 81 | 9.769 | 1304 | 1306 | 1311 | rVV | 214061 | 177329 | 14.59% | 0.727% |
| 82 | 9.839 | 1315 | 1318 | 1323 | rVB | 272259 | 270302 | 22.25% | 1.108% |
| 83 | 10.269 | 1389 | 1391 | 1394 | rVV | 119028 | 99086 | 8.16% | 0.406% |
| 84 | 10.633 | 1450 | 1453 | 1464 | rVV2 | 116328 | 153287 | 12.62% | 0.628% |
| 85 | 10.739 | 1468 | 1471 | 1481 | rVB | 71551 | 93233 | 7.67% | 0.382% |
| 86 | 11.327 | 1568 | 1571 | 1583 | rBV | 227861 | 283386 | 23.32% | 1.161% |
| 87 | 11.716 | 1633 | 1637 | 1640 | rBV | 368258 | 309035 | 25.43% | 1.266% |
| 88 | 12.398 | 1745 | 1753 | 1755 | rBV | 1103461 | 1054408 | 86.78% | 4.320% |
| 89 | 12.421 | 1755 | 1757 | 1763 | rVB | 1491350 | 1215033 | 100.00% | 4.979% |
| 90 | 12.504 | 1768 | 1771 | 1775 | rVB | 177676 | 139942 | 11.52% | 0.573% |
| 91 | 12.545 | 1775 | 1778 | 1784 | rBV2 | 38901 | 78509 | 6.46% | 0.322% |
| 92 | 12.774 | 1815 | 1817 | 1823 | rVB2 | 71998 | 79878 | 6.57% | 0.327% |
| 93 | 12.910 | 1836 | 1840 | 1843 | rBV | 373246 | 344565 | 28.36% | 1.412% |
| 94 | 13.133 | 1875 | 1878 | 1884 | rBV3 | 52510 | 69949 | 5.76% | 0.287% |
| 95 | 13.804 | 1989 | 1992 | 1994 | rBV2 | 78779 | 80160 | 6.60% | 0.328% |
| 96 | 13.974 | 2017 | 2021 | 2030 | rBV | 246592 | 297542 | 24.49% | 1.219% |
| 97 | 14.121 | 2042 | 2046 | 2049 | rBV | 66375 | 80755 | 6.65% | 0.331% |
| 98 | 14.421 | 2095 | 2097 | 2101 | rVB | 80511 | 72235 | 5.95% | 0.296% |
| 99 | 15.051 | 2201 | 2204 | 2207 | rVB | 75673 | 81800 | 6.73% | 0.335% |
| 100 | 15.427 | 2264 | 2268 | 2274 | rVB2 | 148811 | 252199 | 20.76% | 1.033% |

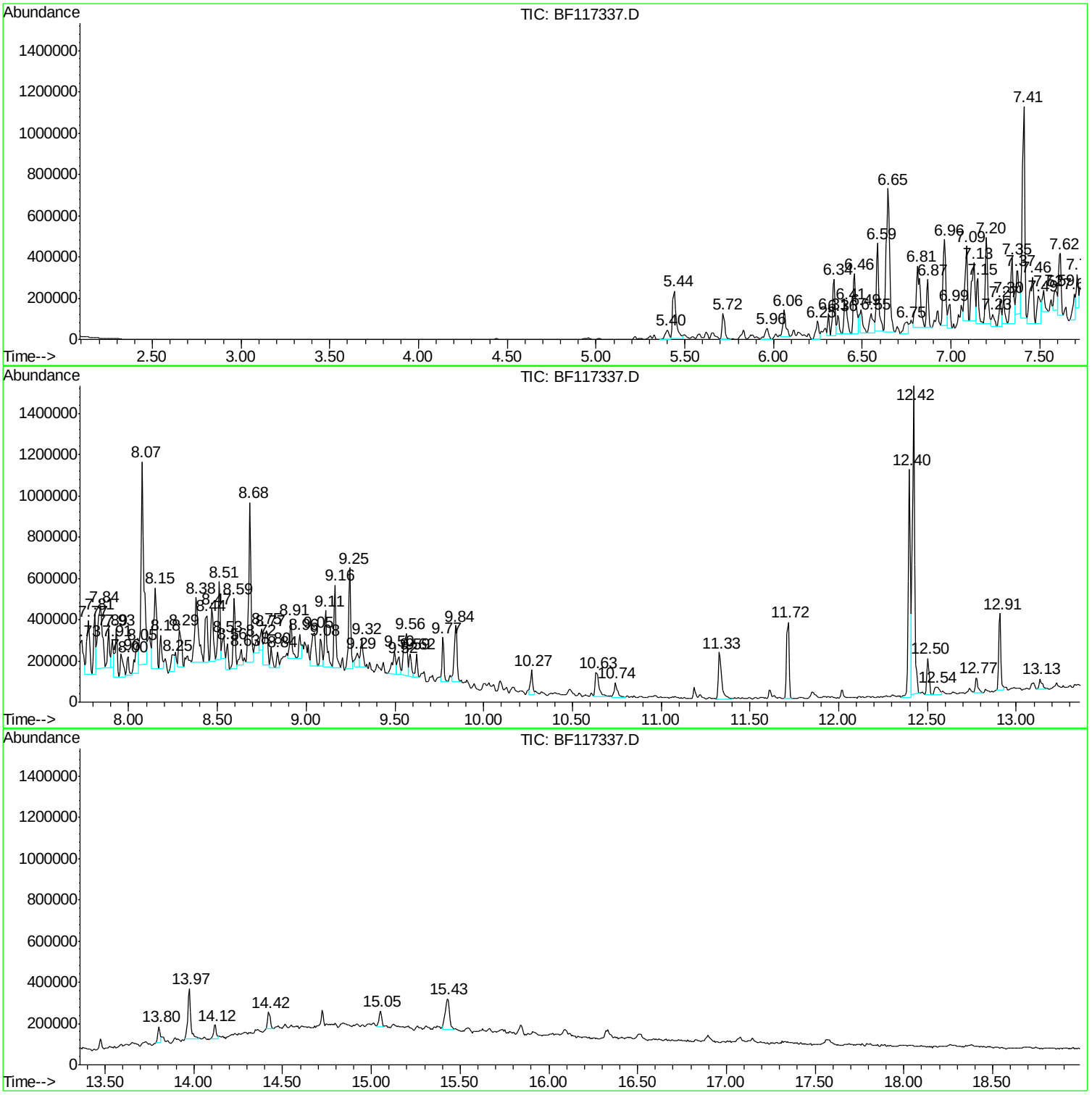
Sum of corrected areas: 24405385

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117337.D
Acq On : 4 Oct 2019 00:38
Operator : JU
Sample : K5140-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
HR-05-100219

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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\BF100319\
Data File : BF117337.D
Acq On : 4 Oct 2019 00:38
Operator : JU
Sample : K5140-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-05-100219

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

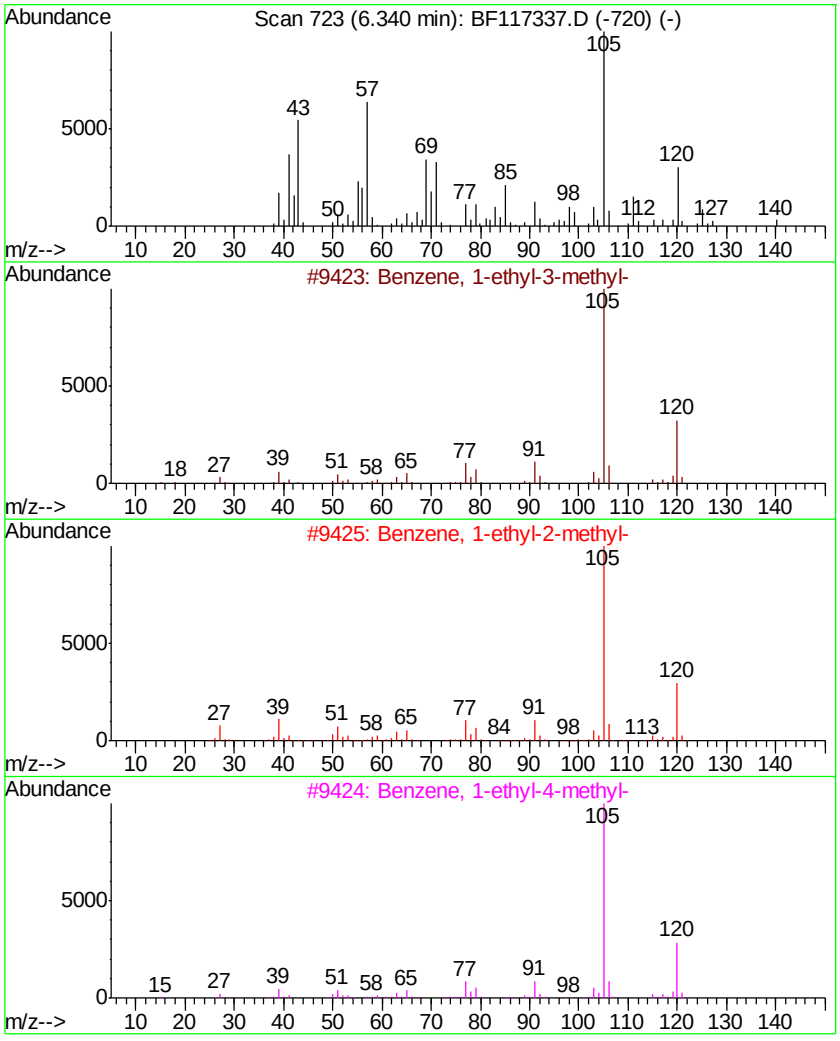
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

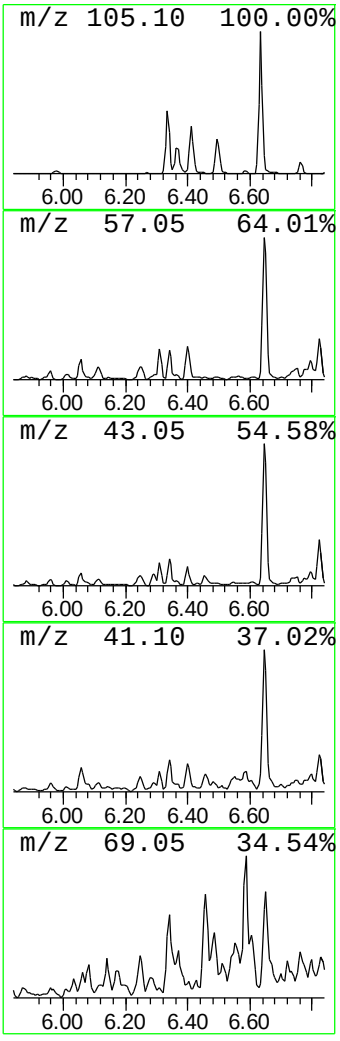
**********

Peak Number 1 Benzene, 1-ethyl-3-methyl- Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.34 | 11.21 ng | 281167 | 1,4-Dichlorobenzene-d4 | 6.81 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzene, 1-ethyl-3-methyl- | 120 | C9H12 | 000620-14-4 | 86 |
| 2 | Benzene, 1-ethyl-2-methyl- | 120 | C9H12 | 000611-14-3 | 83 |
| 3 | Benzene, 1-ethyl-4-methyl- | 120 | C9H12 | 000622-96-8 | 42 |
| 4 | Benzene, 1,2,4-trimethyl- | 120 | C9H12 | 000095-63-6 | 38 |
| 5 | Mesitylene | 120 | C9H12 | 000108-67-8 | 38 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117337.D
Acq On : 4 Oct 2019 00:38
Operator : JU
Sample : K5140-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-05-100219

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

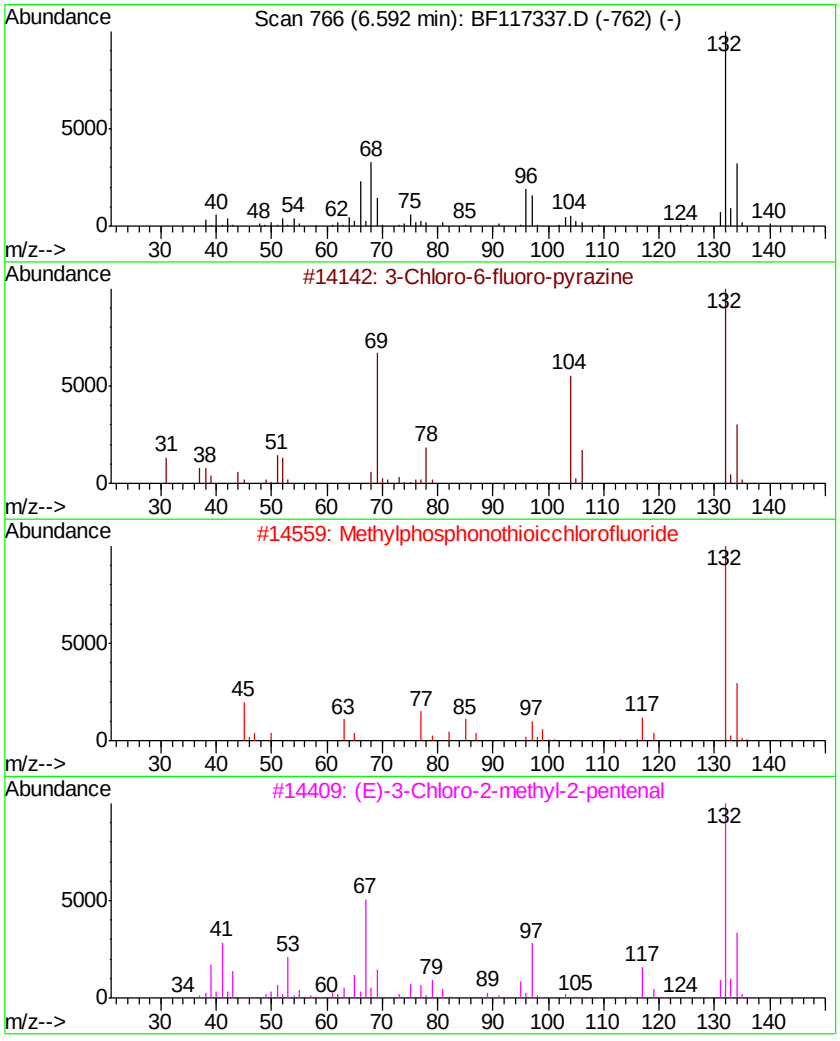
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

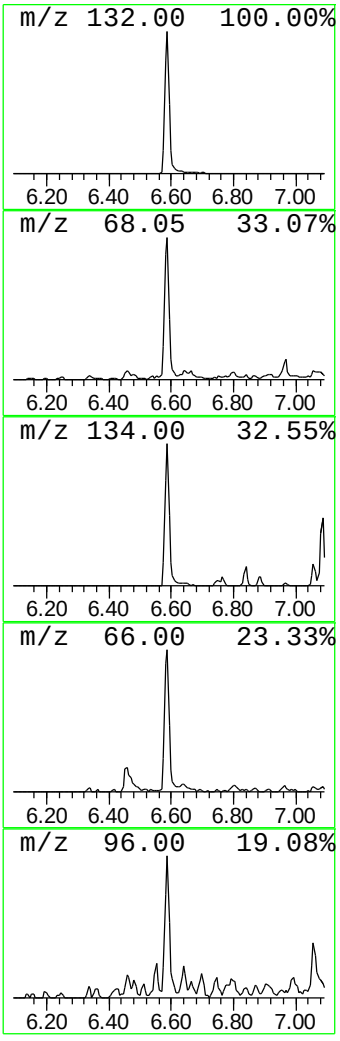
**********

Peak Number 2 unknown6.59 Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.59 | 17.58 ng | 440848 | 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 | Methylphosphonothioicchlorofluoride | 132 | CH3ClFPS | 027127-27-1 | 27 |
| 3 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 25 |
| 4 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |
| 5 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
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Operator : JU
Sample : K5140-01 2X
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ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-05-100219

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

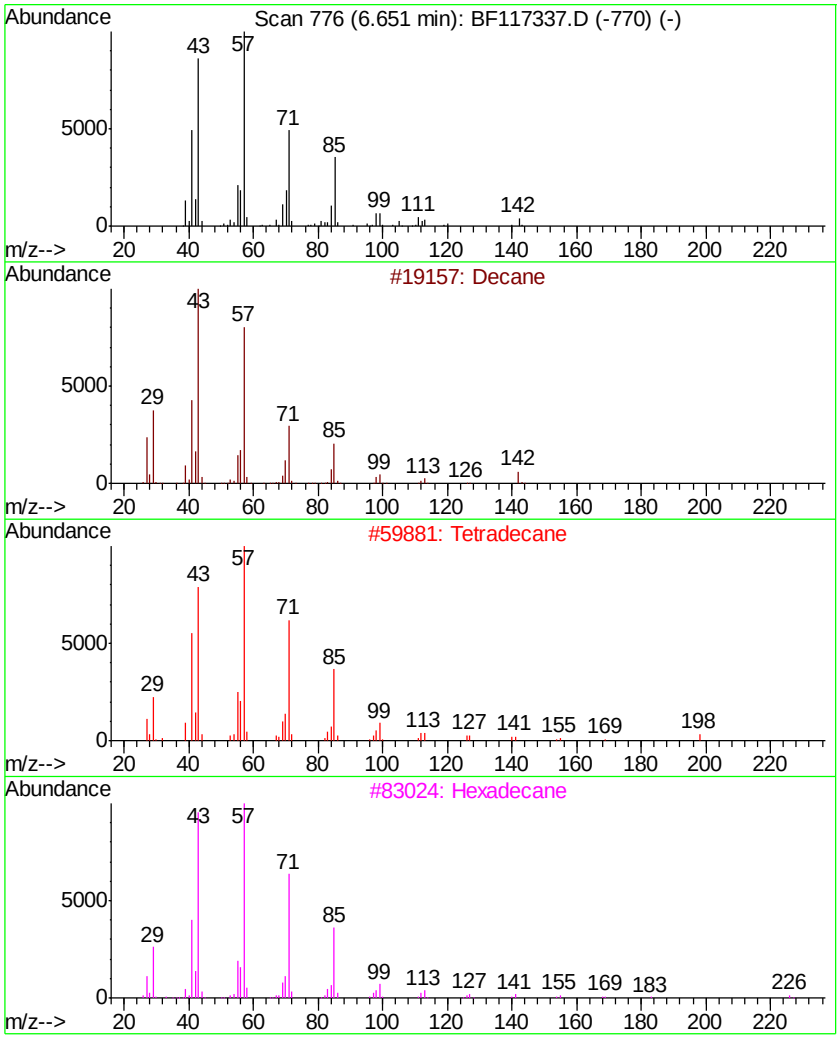
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

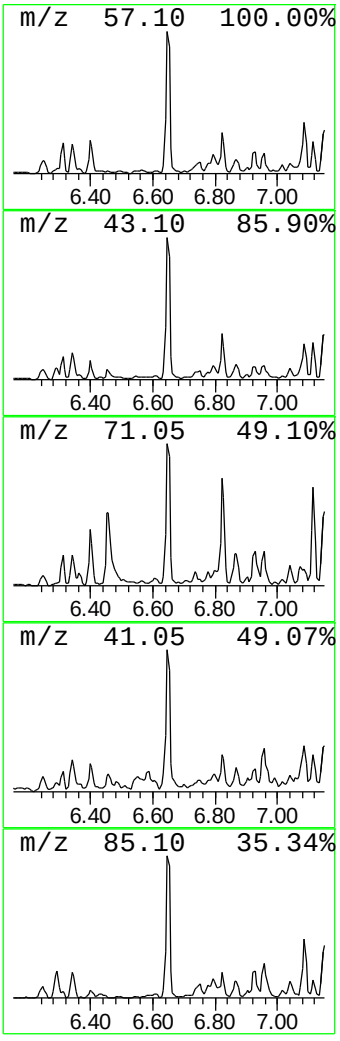
**********

Peak Number 3 Decane Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.65 | 37.77 ng | 947194 | 1,4-Dichlorobenzene-d4 | 6.81 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Decane | 142 | C10H22 | 000124-18-5 | 93 |
| 2 | Tetradecane | 198 | C14H30 | 000629-59-4 | 78 |
| 3 | Hexadecane | 226 | C16H34 | 000544-76-3 | 72 |
| 4 | Undecane | 156 | C11H24 | 001120-21-4 | 64 |
| 5 | Tridecane | 184 | C13H28 | 000629-50-5 | 64 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117337.D
Acq On : 4 Oct 2019 00:38
Operator : JU
Sample : K5140-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-05-100219

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

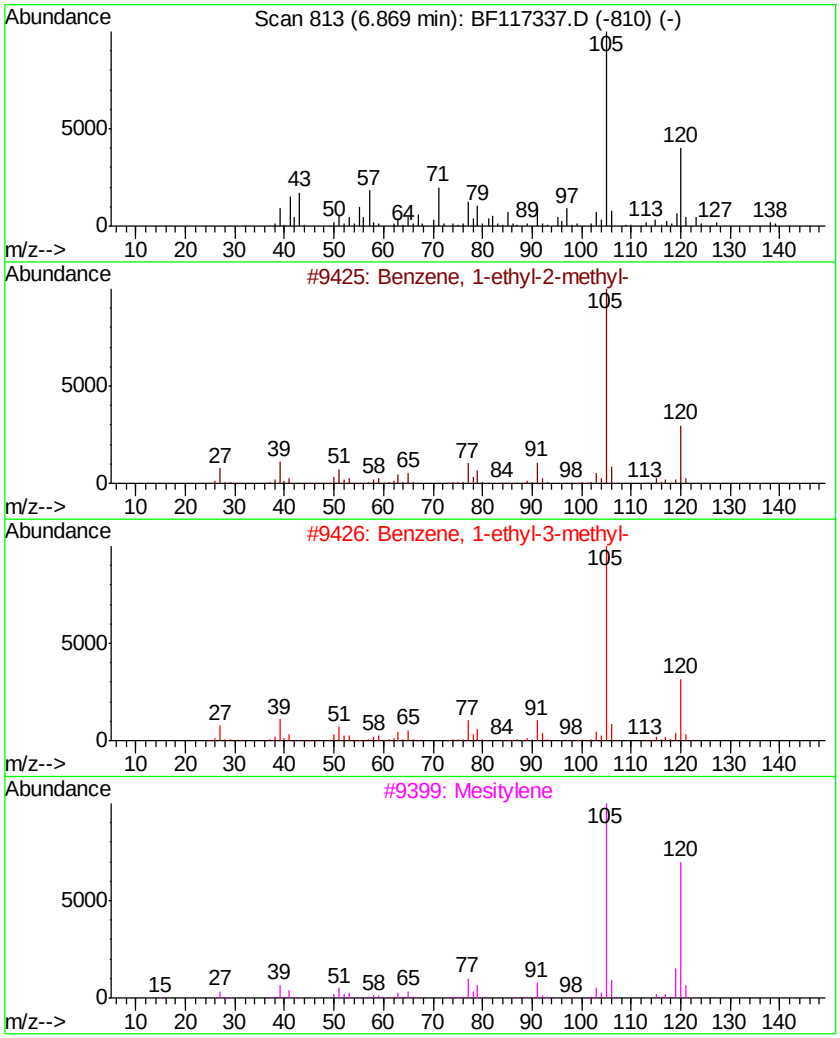
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

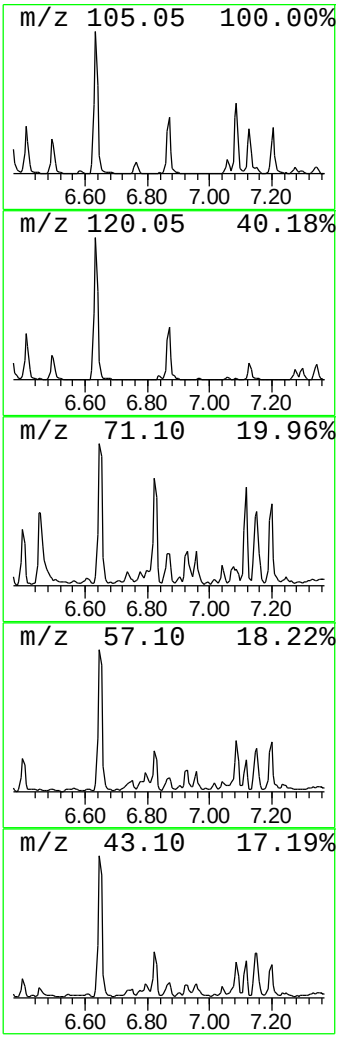
**********

Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 20

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.87 | 8.21 ng | 205811 | 1,4-Dichlorobenzene-d4 | 6.81 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzene, 1-ethyl-2-methyl- | 120 | C9H12 | 000611-14-3 | 64 |
| 2 | Benzene, 1-ethyl-3-methyl- | 120 | C9H12 | 000620-14-4 | 64 |
| 3 | Mesitylene | 120 | C9H12 | 000108-67-8 | 64 |
| 4 | Benzene, 1-ethyl-4-methyl- | 120 | C9H12 | 000622-96-8 | 64 |
| 5 | Benzene, 1,2,3-trimethyl- | 120 | C9H12 | 000526-73-8 | 60 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117337.D
Acq On : 4 Oct 2019 00:38
Operator : JU
Sample : K5140-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-05-100219

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

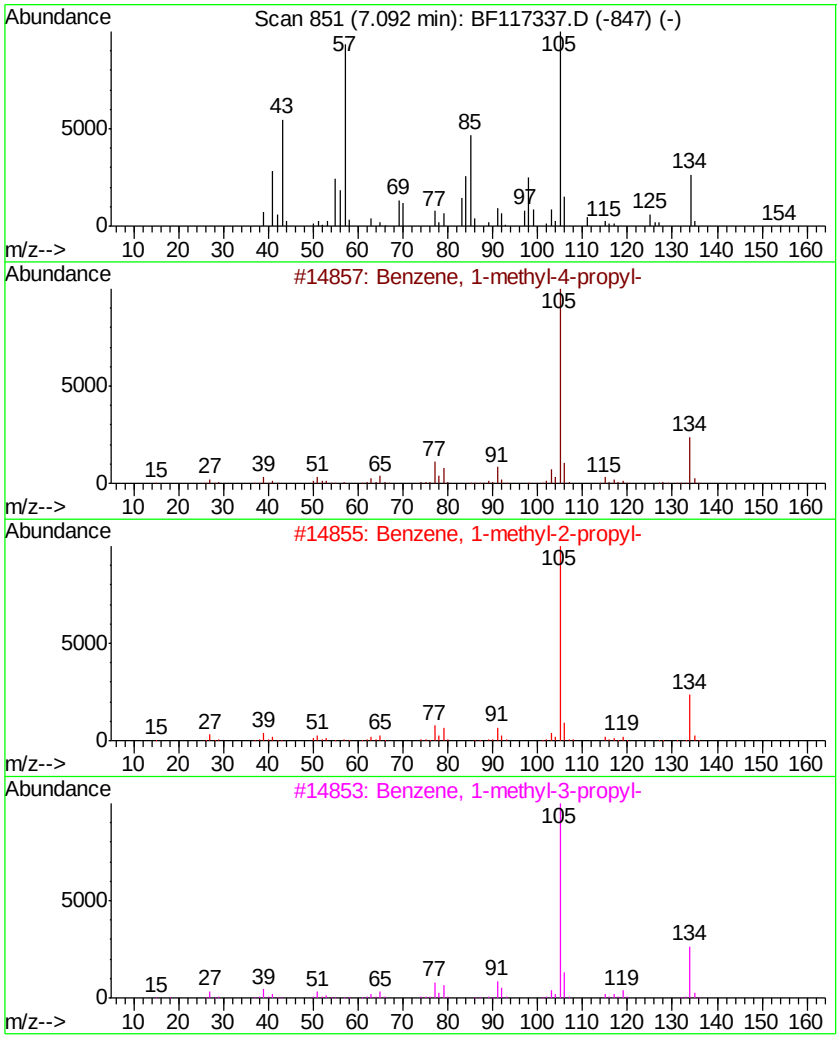
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

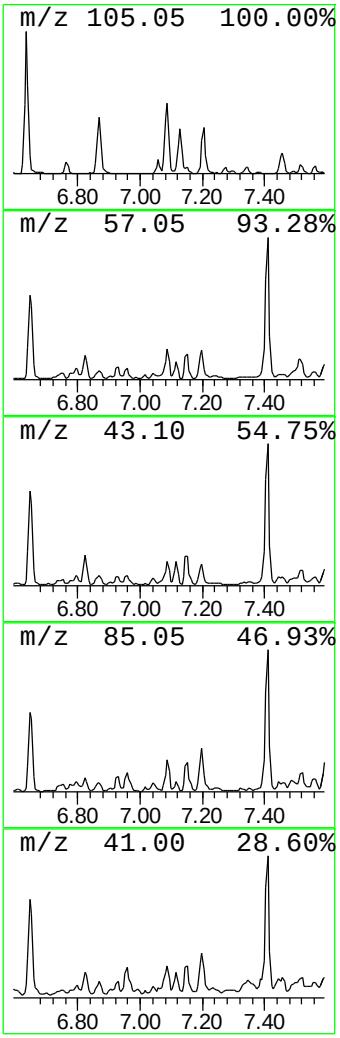
**********

Peak Number 6 Benzene, 1-methyl-4-propyl- Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.09 | 12.78 ng | 320575 | 1,4-Dichlorobenzene-d4 | 6.81 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzene, 1-methyl-4-propyl- | 134 | C10H14 | 001074-55-1 | 86 |
| 2 | Benzene, 1-methyl-2-propyl- | 134 | C10H14 | 001074-17-5 | 55 |
| 3 | Benzene, 1-methyl-3-propyl- | 134 | C10H14 | 001074-43-7 | 55 |
| 4 | Benzene, (1-methylpropyl)- | 134 | C10H14 | 000135-98-8 | 45 |
| 5 | Benzeneacetaldehyde, .alpha.-met... | 134 | C9H10O | 000093-53-8 | 38 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117337.D
Acq On : 4 Oct 2019 00:38
Operator : JU
Sample : K5140-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-05-100219

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

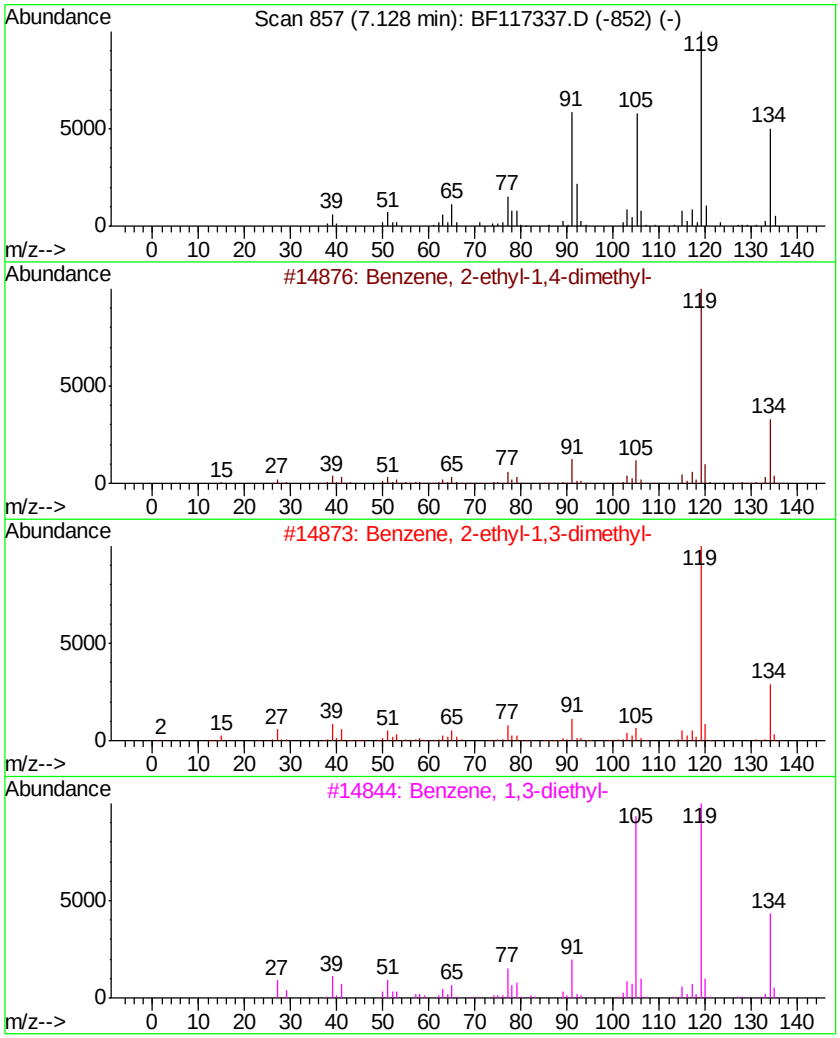
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

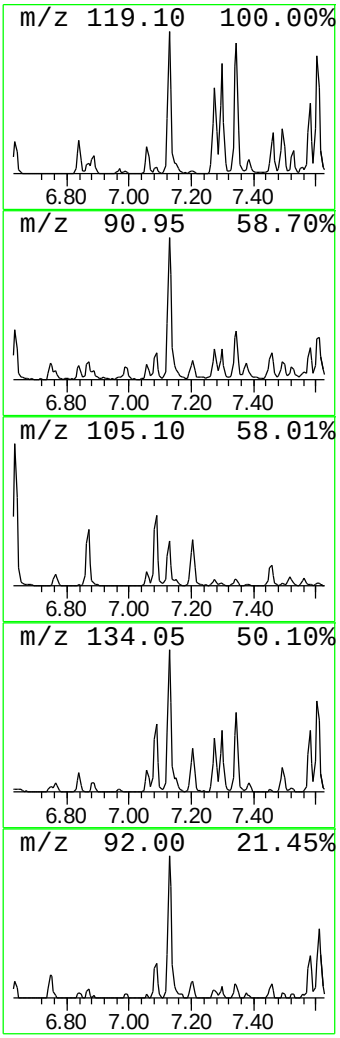
**********

Peak Number 7 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.13 | 13.74 ng | 344466 | 1,4-Dichlorobenzene-d4 | 6.81 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzene, 2-ethyl-1,4-dimethyl- | 134 | C10H14 | 001758-88-9 | 91 |
| 2 | Benzene, 2-ethyl-1,3-dimethyl- | 134 | C10H14 | 002870-04-4 | 90 |
| 3 | Benzene, 1,3-diethyl- | 134 | C10H14 | 000141-93-5 | 90 |
| 4 | Benzene, 1-ethyl-2,3-dimethyl- | 134 | C10H14 | 000933-98-2 | 90 |
| 5 | Benzene, 1,4-diethyl- | 134 | C10H14 | 000105-05-5 | 90 |



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Data File : BF117337.D
Acq On : 4 Oct 2019 00:38
Operator : JU
Sample : K5140-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-05-100219

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

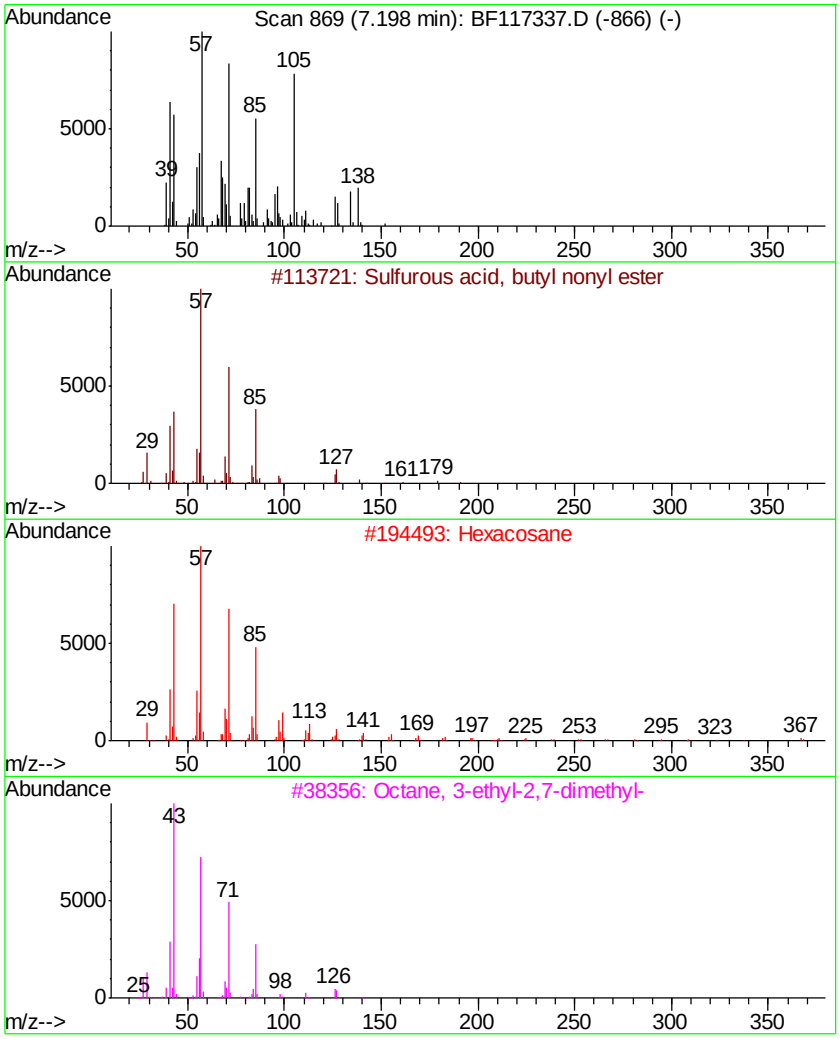
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

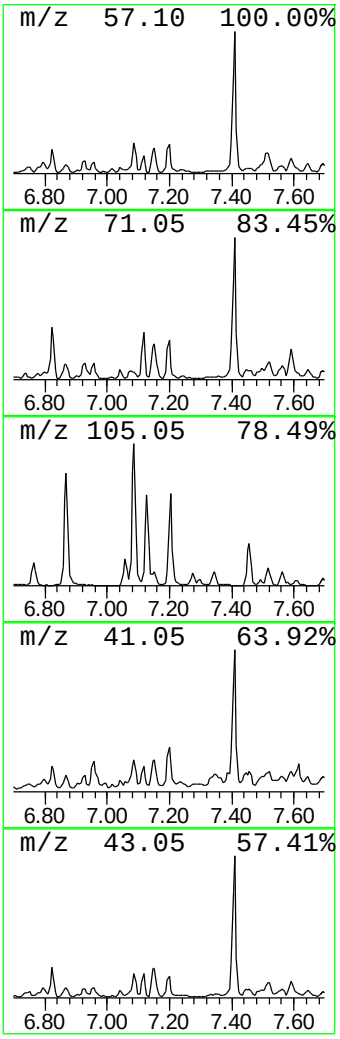
**********

Peak Number 8 unknown7.20 Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.20 | 16.62 ng | 416836 | 1,4-Dichlorobenzene-d4 | 6.81 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Sulfurous acid, butyl nonyl ester | 264 | C13H28O3S | 1000309-17-6 | 43 |
| 2 | Hexacosane | 366 | C26H54 | 000630-01-3 | 43 |
| 3 | Octane, 3-ethyl-2,7-dimethyl- | 170 | C12H26 | 062183-55-5 | 43 |
| 4 | Cyclohexanol, 5-methyl-2-(1-meth... | 156 | C10H20O | 000491-02-1 | 43 |
| 5 | Hexane, 2,3,4-trimethyl- | 128 | C9H20 | 000921-47-1 | 43 |



# Library Search Compound Report

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Data File : BF117337.D
Acq On : 4 Oct 2019 00:38
Operator : JU
Sample : K5140-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-05-100219

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

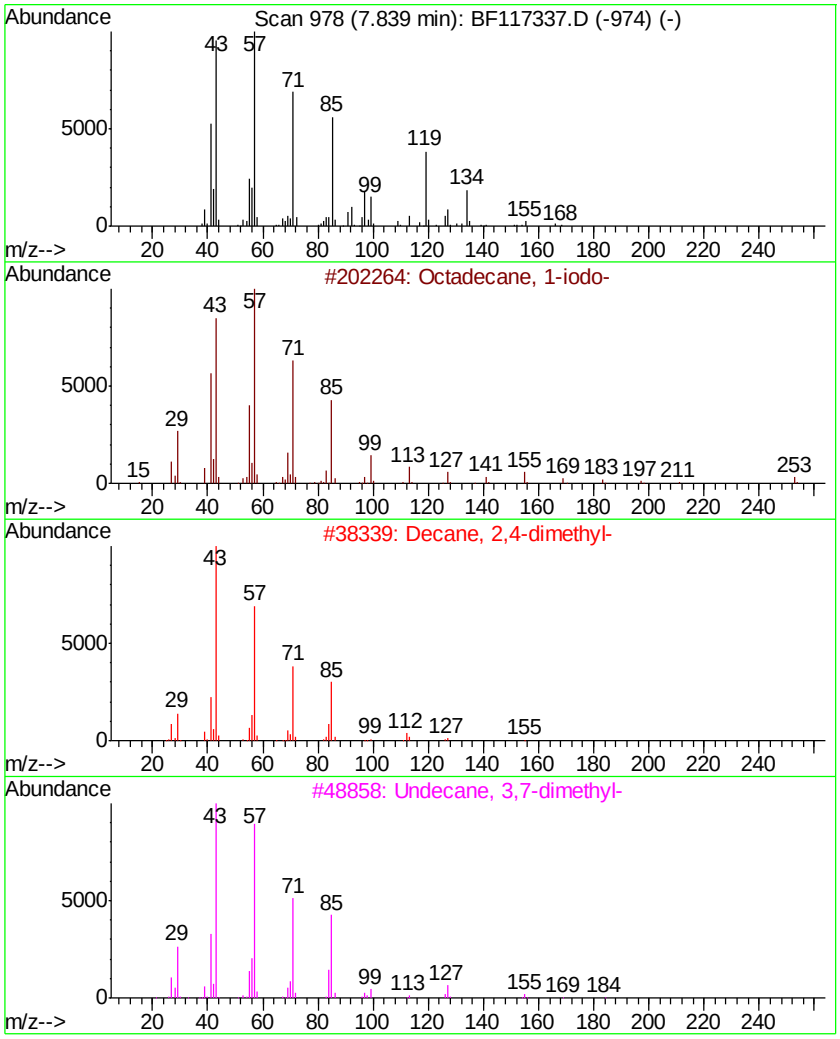
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

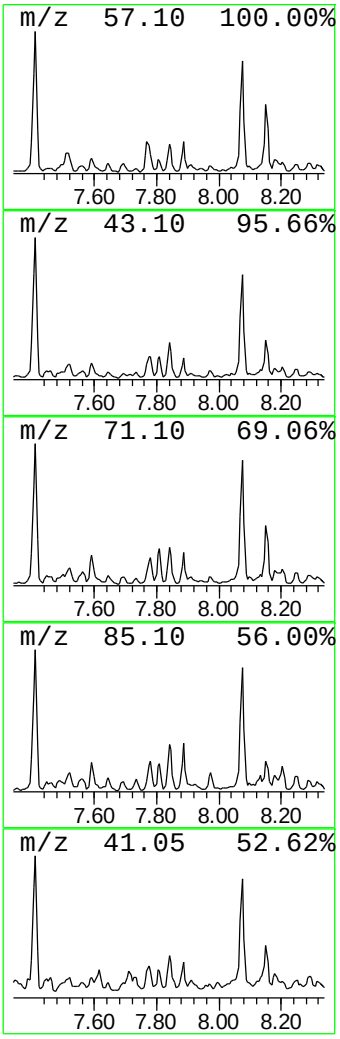
**********

Peak Number 9 unknown7.84 Concentration Rank 19

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.84 | 9.41 ng | 556955 | Naphthalene-d8 | 8.09 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecane, 1-iodo- | 380 | C18H37I | 000629-93-6 | 47 |
| 2 | Decane, 2,4-dimethyl- | 170 | C12H26 | 002801-84-5 | 43 |
| 3 | Undecane, 3,7-dimethyl- | 184 | C13H28 | 017301-29-0 | 43 |
| 4 | Hexane, 2,3,4-trimethyl- | 128 | C9H20 | 000921-47-1 | 43 |
| 5 | 1-Iodo-2-methylnonane | 268 | C10H21I | 1000101-47-9 | 38 |



# Library Search Compound Report

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Data File : BF117337.D
Acq On : 4 Oct 2019 00:38
Operator : JU
Sample : K5140-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-05-100219

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

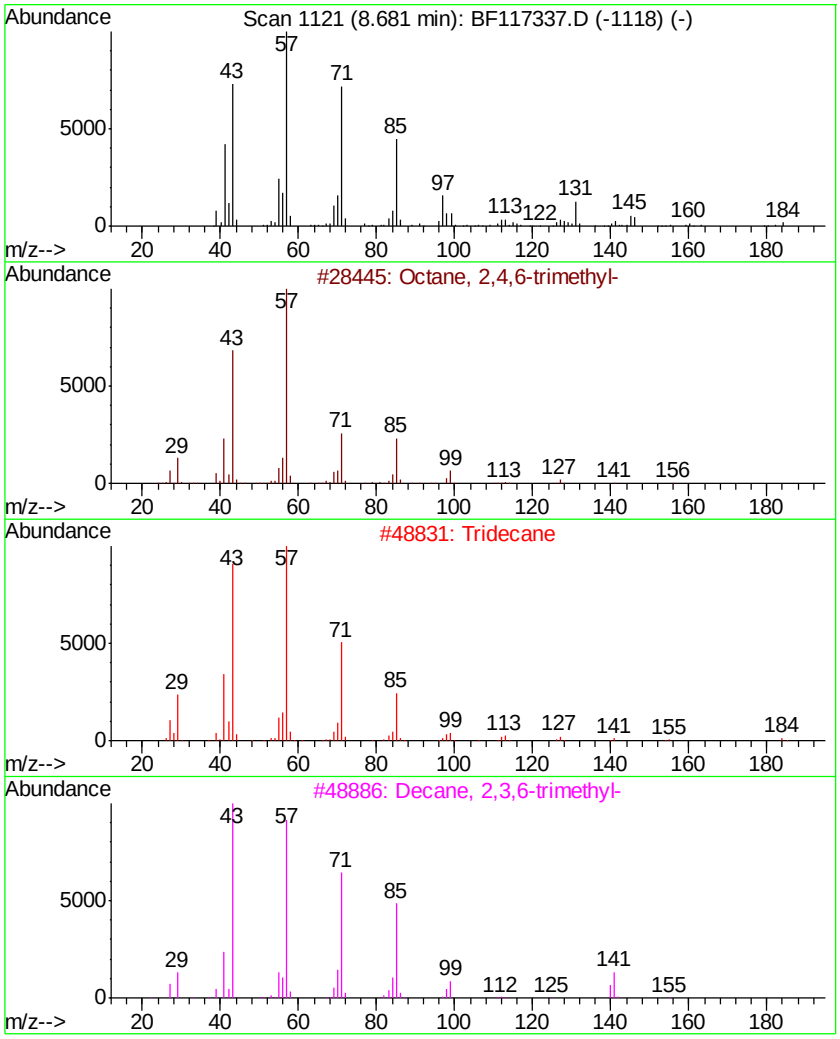
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

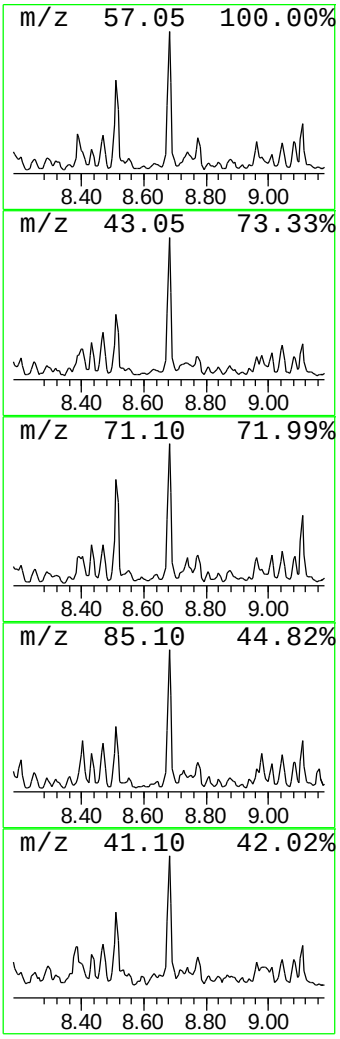
**********

Peak Number 10 Octane, 2,4,6-trimethyl- Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.68 | 11.62 ng | 687903 | Naphthalene-d8 | 8.09 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octane, 2,4,6-trimethyl- | 156 | C11H24 | 062016-37-9 | 64 |
| 2 | Tridecane | 184 | C13H28 | 000629-50-5 | 64 |
| 3 | Decane, 2,3,6-trimethyl- | 184 | C13H28 | 062238-12-4 | 59 |
| 4 | Tetradecane | 198 | C14H30 | 000629-59-4 | 59 |
| 5 | 1-Iodo-2-methylnonane | 268 | C10H21I | 1000101-47-9 | 50 |



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Data File : BF117337.D
Acq On : 4 Oct 2019 00:38
Operator : JU
Sample : K5140-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-05-100219

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

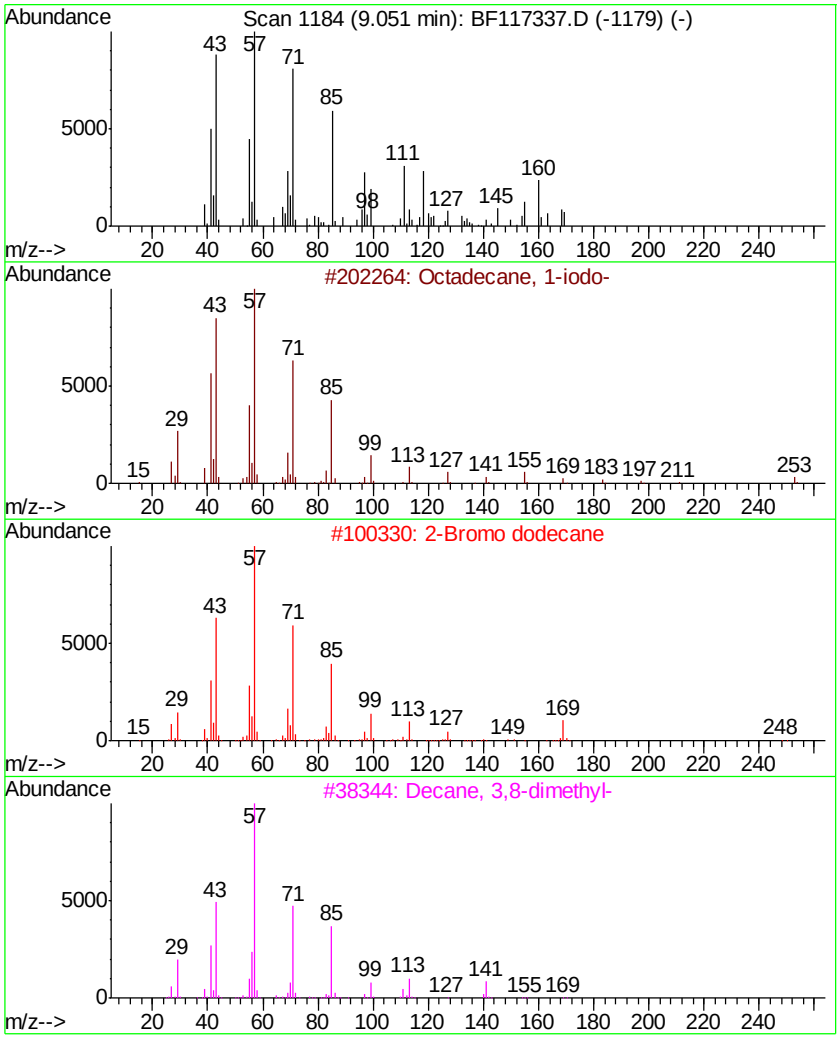
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

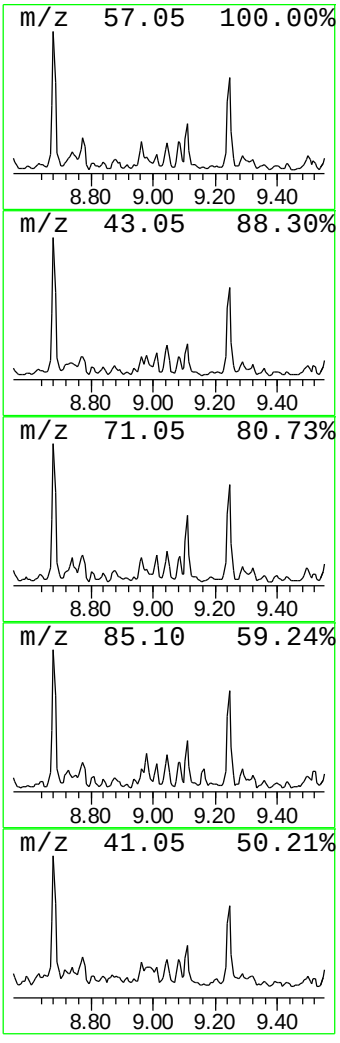
**********

Peak Number 11 Octadecane, 1-iodo- Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.05 | 16.85 ng | 227681 | Acenaphthene-d10 | 9.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecane, 1-iodo- | 380 | C18H37I | 000629-93-6 | 64 |
| 2 | 2-Bromo dodecane | 248 | C12H25Br | 013187-99-0 | 64 |
| 3 | Decane, 3,8-dimethyl- | 170 | C12H26 | 017312-55-9 | 64 |
| 4 | 1-Iodo-2-methylnonane | 268 | C10H21I | 1000101-47-9 | 64 |
| 5 | Decane, 2,3,5,8-tetramethyl- | 198 | C14H30 | 192823-15-7 | 59 |



# Library Search Compound Report

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Data File : BF117337.D
Acq On : 4 Oct 2019 00:38
Operator : JU
Sample : K5140-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-05-100219

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

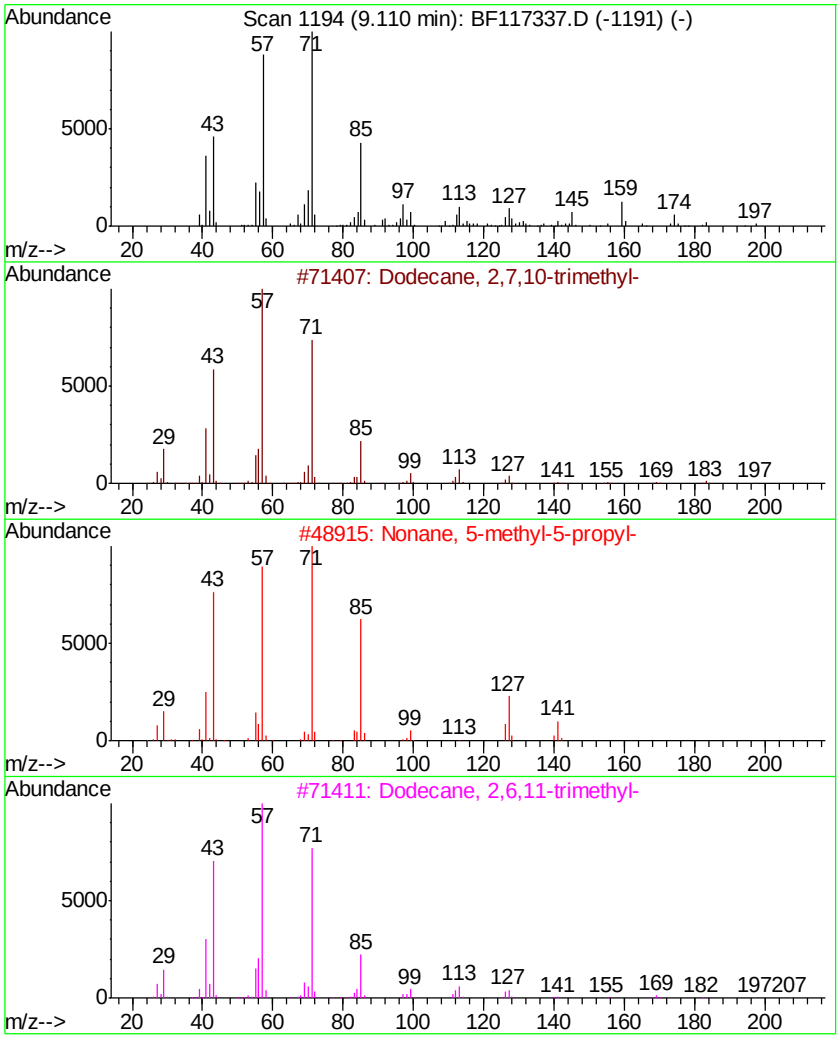
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

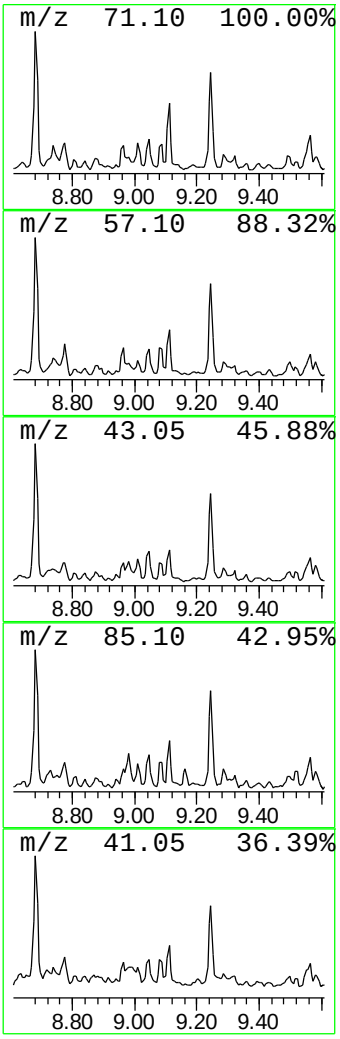
**********

Peak Number 12 Dodecane, 2,7,10-trimethyl- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.11 | 21.76 ng | 294118 | Acenaphthene-d10 | 9.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dodecane, 2,7,10-trimethyl- | 212 | C15H32 | 074645-98-0 | 58 |
| 2 | Nonane, 5-methyl-5-propyl- | 184 | C13H28 | 017312-75-3 | 53 |
| 3 | Dodecane, 2,6,11-trimethyl- | 212 | C15H32 | 031295-56-4 | 53 |
| 4 | Dodecane, 2,6,10-trimethyl- | 212 | C15H32 | 003891-98-3 | 49 |
| 5 | Octane, 2,6-dimethyl- | 142 | C10H22 | 002051-30-1 | 49 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117337.D
Acq On : 4 Oct 2019 00:38
Operator : JU
Sample : K5140-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-05-100219

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

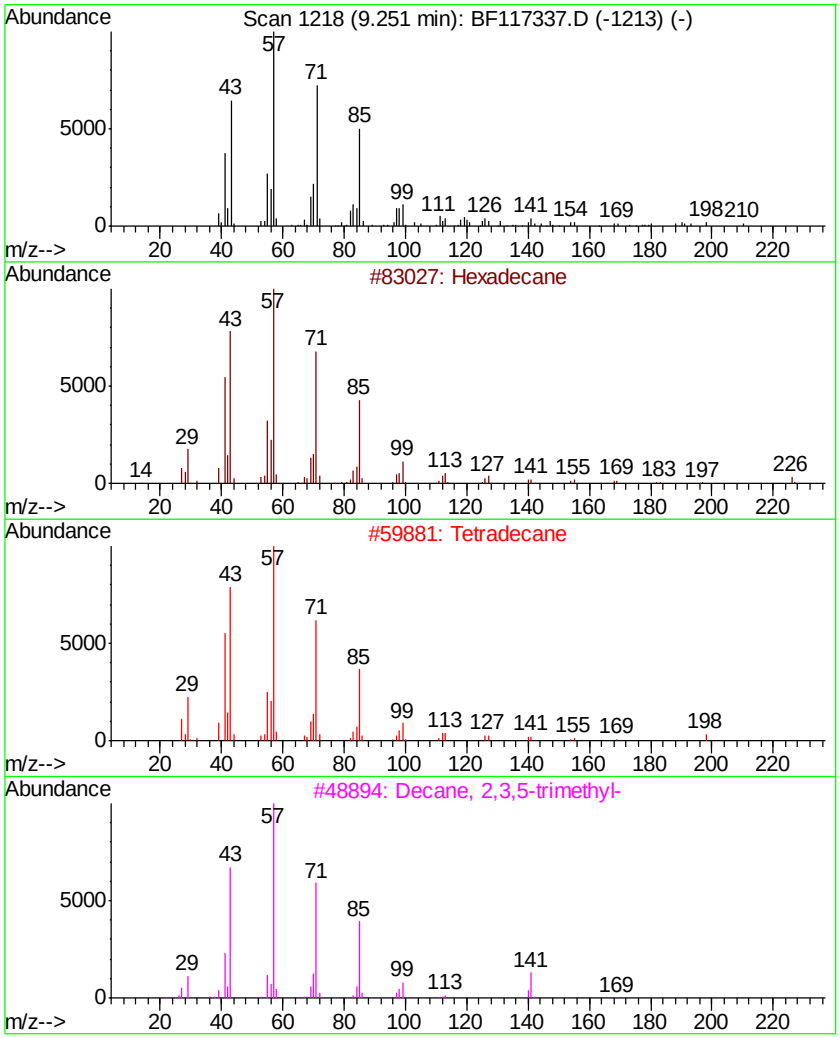
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

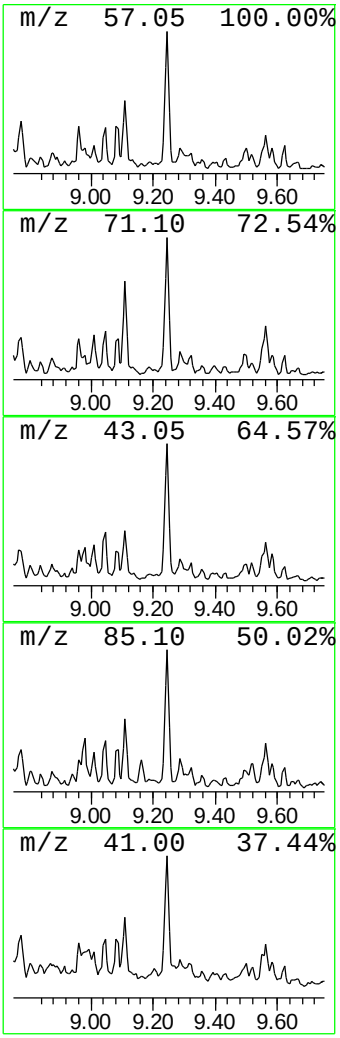
**********

Peak Number 13 Hexadecane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.25 | 32.91 ng | 444762 | Acenaphthene-d10 | 9.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane | 226 | C16H34 | 000544-76-3 | 90 |
| 2 | Tetradecane | 198 | C14H30 | 000629-59-4 | 86 |
| 3 | Decane, 2,3,5-trimethyl- | 184 | C13H28 | 062238-11-3 | 83 |
| 4 | Heneicosane | 296 | C21H44 | 000629-94-7 | 72 |
| 5 | Sulfurous acid, hexyl pentyl ester | 236 | C11H24O3S | 1000309-14-1 | 64 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117337.D
Acq On : 4 Oct 2019 00:38
Operator : JU
Sample : K5140-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-05-100219

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

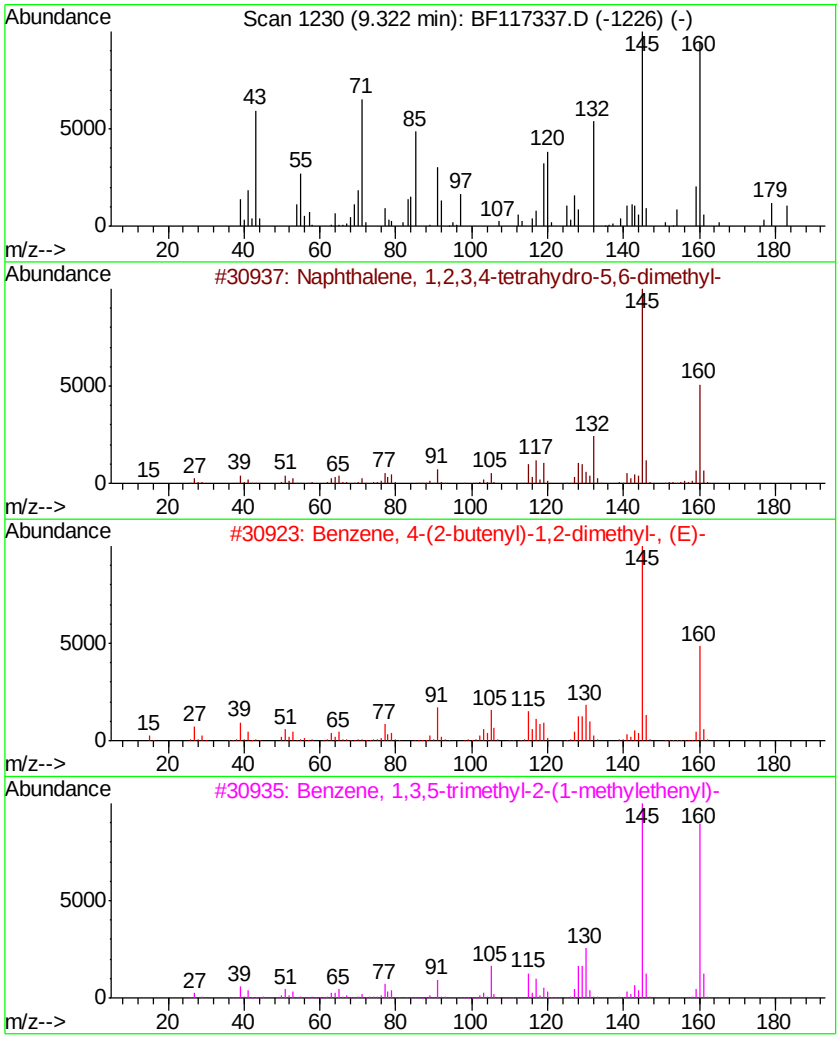
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

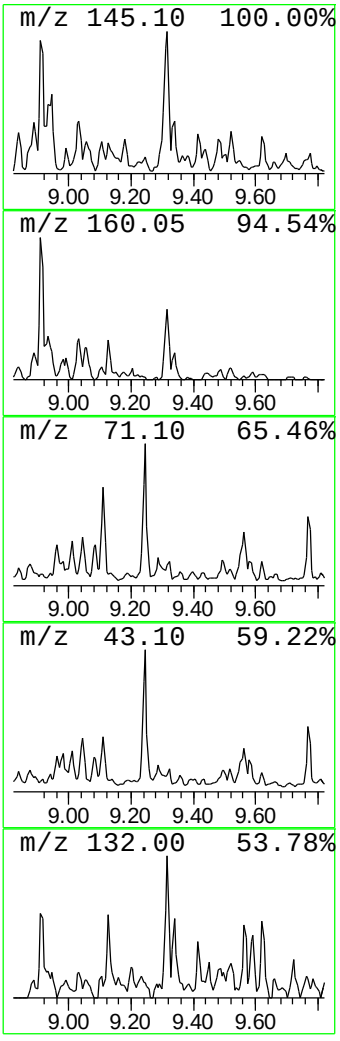
**********

Peak Number 14 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 18

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.32 | 9.83 ng | 132848 | Acenaphthene-d10 | 9.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Naphthalene, 1,2,3,4-tetrahydro-... | 160 | C12H16 | 020027-77-4 | 91 |
| 2 | Benzene, 4-(2-butenyl)-1,2-dimet... | 160 | C12H16 | 054340-86-2 | 87 |
| 3 | Benzene, 1,3,5-trimethyl-2-(1-me... | 160 | C12H16 | 014679-13-1 | 81 |
| 4 | Naphthalene, 1,2,3,4-tetrahydro-... | 160 | C12H16 | 021693-54-9 | 80 |
| 5 | Naphthalene, 1,2,3,4-tetrahydro-... | 160 | C12H16 | 001076-61-5 | 76 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117337.D
Acq On : 4 Oct 2019 00:38
Operator : JU
Sample : K5140-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-05-100219

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

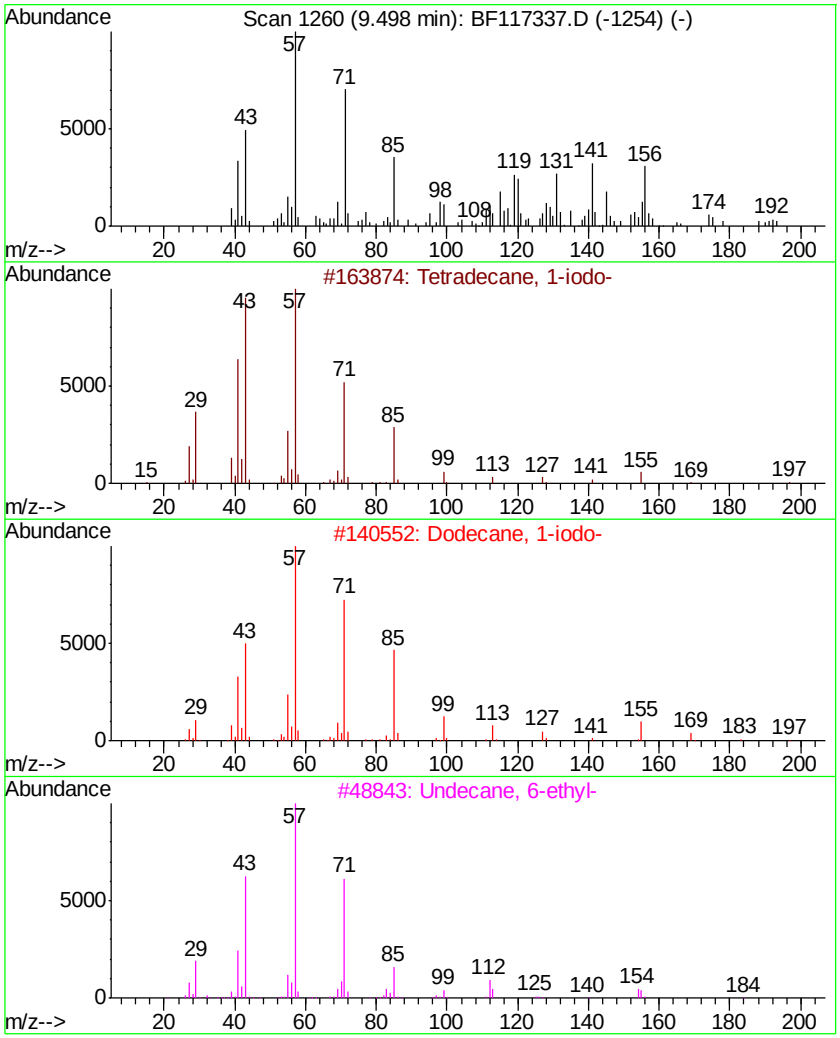
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

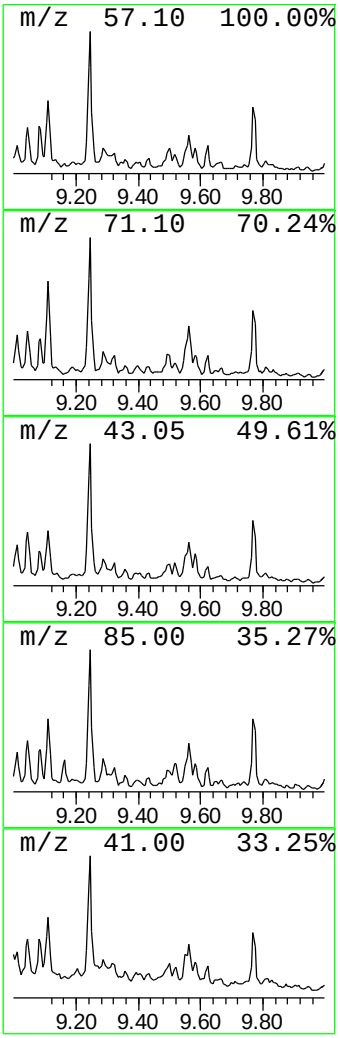
**********

Peak Number 15 unknown9.50 Concentration Rank 15

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.50 | 11.51 ng | 155578 | Acenaphthene-d10 | 9.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetradecane, 1-iodo- | 324 | C14H29I | 019218-94-1 | 27 |
| 2 | Dodecane, 1-iodo- | 296 | C12H25I | 004292-19-7 | 22 |
| 3 | Undecane, 6-ethyl- | 184 | C13H28 | 017312-60-6 | 22 |
| 4 | Tridecane, 1-iodo- | 310 | C13H27I | 035599-77-0 | 22 |
| 5 | 9-Heptadecanone | 254 | C17H34O | 000540-08-9 | 22 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117337.D
Acq On : 4 Oct 2019 00:38
Operator : JU
Sample : K5140-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-05-100219

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

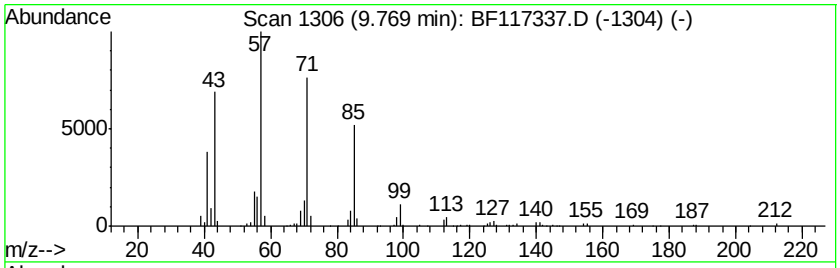
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

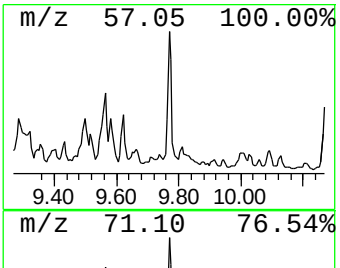
**********

Peak Number 16 Decane, 2,3,5-trimethyl- Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.77 | 13.12 ng | 177329 | Acenaphthene-d10 | 9.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Decane, 2,3,5-trimethyl- | 184 | C13H28 | 062238-11-3 | 90 |
| 2 | Sulfurous acid, 2-propyl tridecy... | 306 | C16H34O3S | 1000309-12-4 | 78 |
| 3 | Nonane, 5-(2-methylpropyl)- | 184 | C13H28 | 062185-53-9 | 72 |
| 4 | Bacchotricuneatin c | 342 | C20H22O5 | 066563-30-2 | 72 |
| 5 | Sulfurous acid, decyl 2-propyl e... | 264 | C13H28O3S | 1000309-12-1 | 64 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117337.D
Acq On : 4 Oct 2019 00:38
Operator : JU
Sample : K5140-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-05-100219

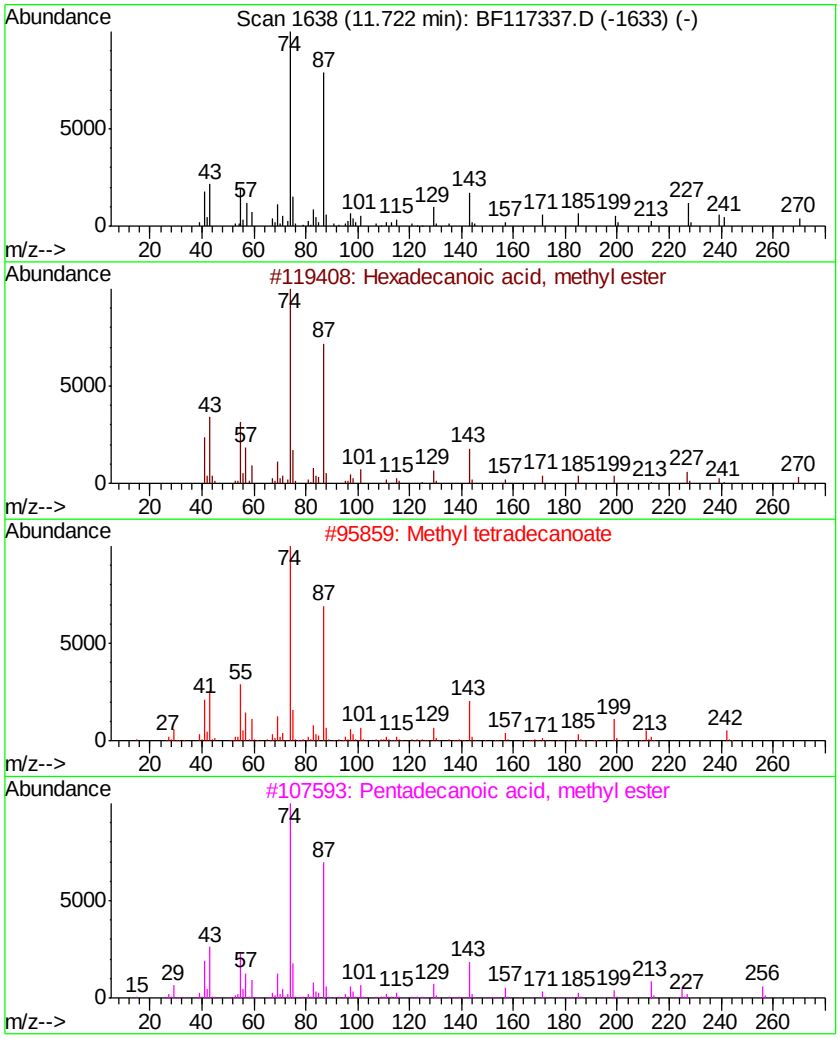
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

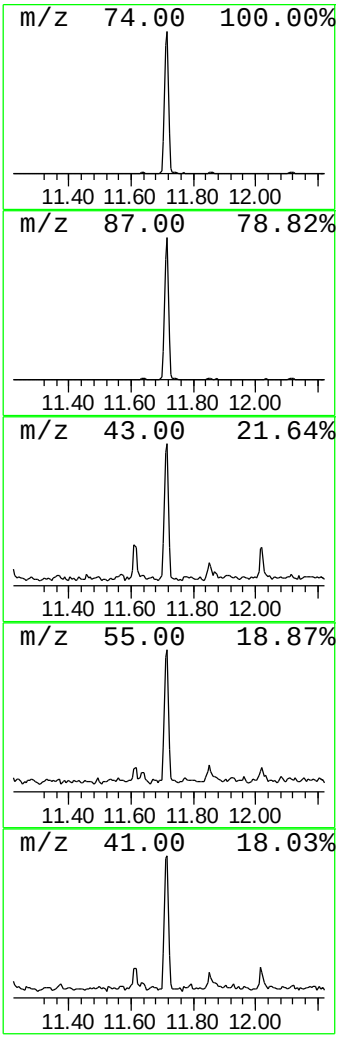
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 17 Hexadecanoic acid, methyl e... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.72 | 21.81 ng | 309035 | Phenanthrene-d10 | 11.33 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecanoic acid, methyl ester | 270 | C17H34O2 | 000112-39-0 | 97 |
| 2 | Methyl tetradecanoate | 242 | C15H30O2 | 000124-10-7 | 86 |
| 3 | Pentadecanoic acid, methyl ester | 256 | C16H32O2 | 007132-64-1 | 86 |
| 4 | Tridecanoic acid, methyl ester | 228 | C14H28O2 | 001731-88-0 | 80 |
| 5 | Pentadecanoic acid, 14-methyl-, ... | 270 | C17H34O2 | 005129-60-2 | 78 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117337.D
Acq On : 4 Oct 2019 00:38
Operator : JU
Sample : K5140-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-05-100219

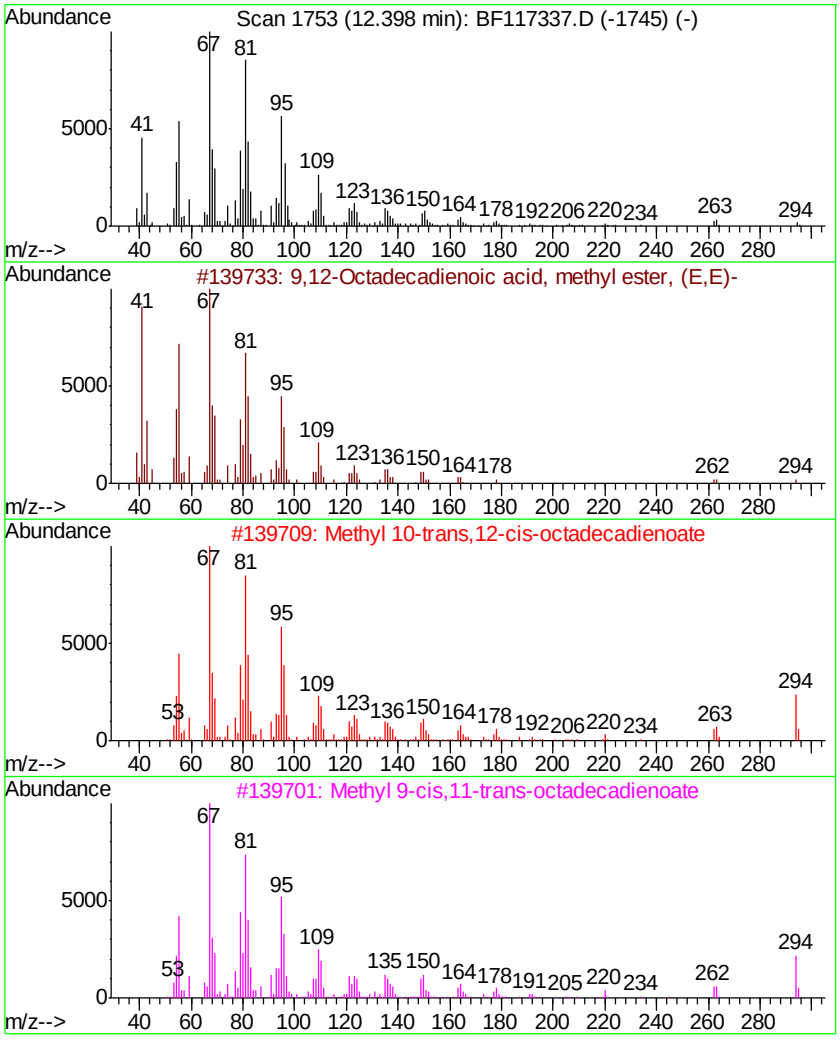
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

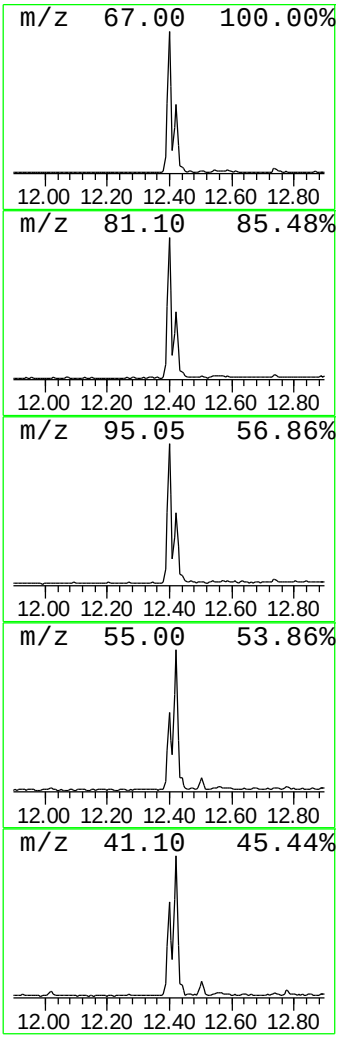
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 18 9,12-Octadecadienoic acid, ... Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.40 | 74.42 ng | 1054410 | Phenanthrene-d10 | 11.33 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9,12-Octadecadienoic acid, methy... | 294 | C19H34O2 | 002566-97-4 | 99 |
| 2 | Methyl 10-trans,12-cis-octadecad... | 294 | C19H34O2 | 1000336-44-2 | 99 |
| 3 | Methyl 9-cis,11-trans-octadecadi... | 294 | C19H34O2 | 1000336-44-0 | 99 |
| 4 | 10,13-Octadecadienoic acid, meth... | 294 | C19H34O2 | 056554-62-2 | 96 |
| 5 | 9,12-Octadecadienoic acid (Z,Z)-... | 294 | C19H34O2 | 000112-63-0 | 96 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117337.D
Acq On : 4 Oct 2019 00:38
Operator : JU
Sample : K5140-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-05-100219

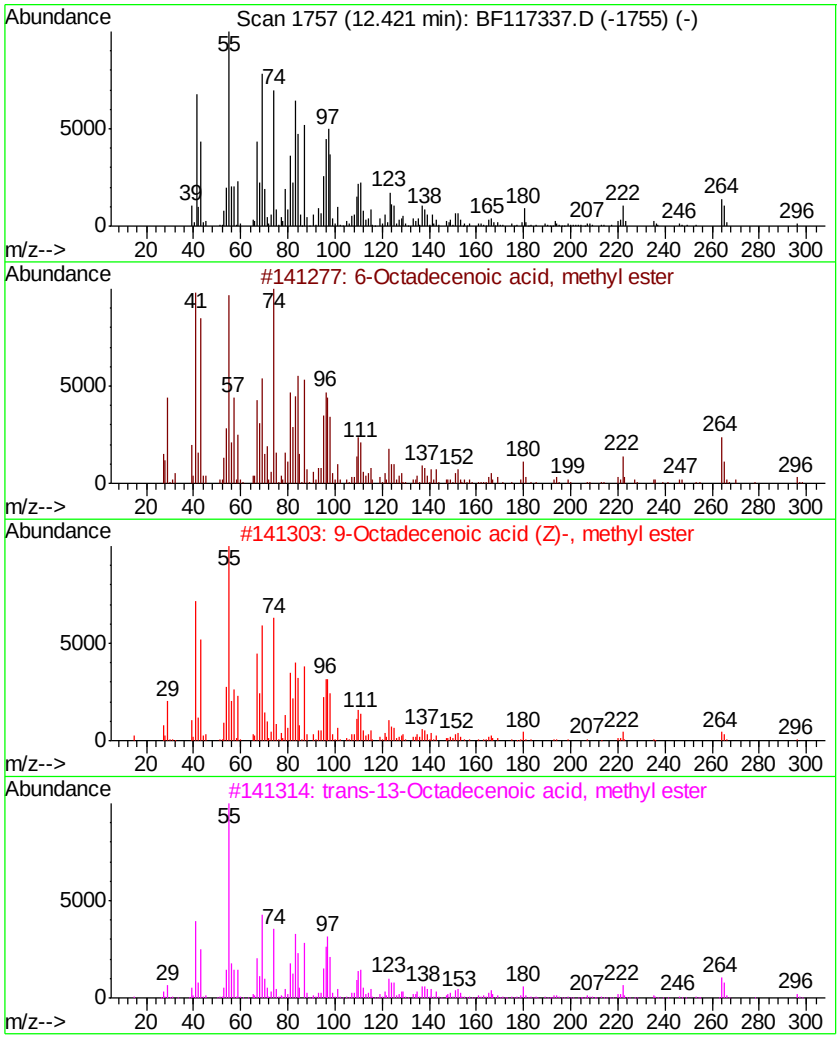
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

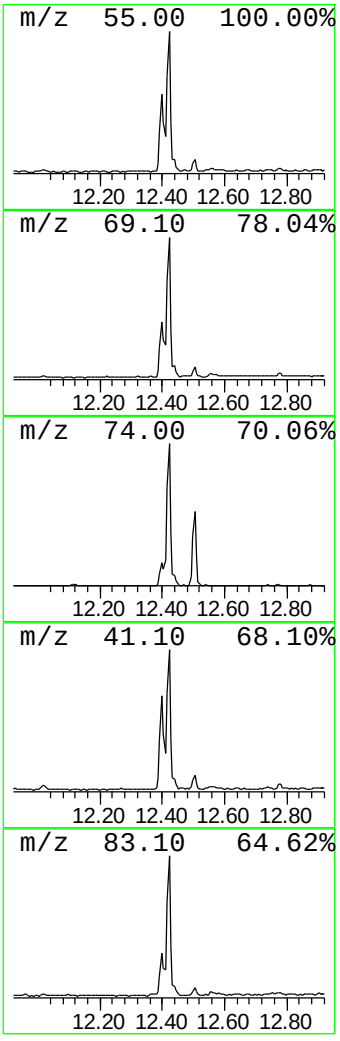
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 19 6-Octadecenoic acid, methyl... Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.42 | 85.75 ng | 1215030 | Phenanthrene-d10 | 11.33 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 6-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 052355-31-4 | 99 |
| 2 | 9-Octadecenoic acid (Z)-, methyl... | 296 | C19H36O2 | 000112-62-9 | 99 |
| 3 | trans-13-Octadecenoic acid, meth... | 296 | C19H36O2 | 1000333-61-3 | 98 |
| 4 | cis-13-Octadecenoic acid, methyl... | 296 | C19H36O2 | 1000333-58-3 | 97 |
| 5 | 7-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 057396-98-2 | 96 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100319\
Data File : BF117337.D
Acq On : 4 Oct 2019 00:38
Operator : JU
Sample : K5140-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-05-100219

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

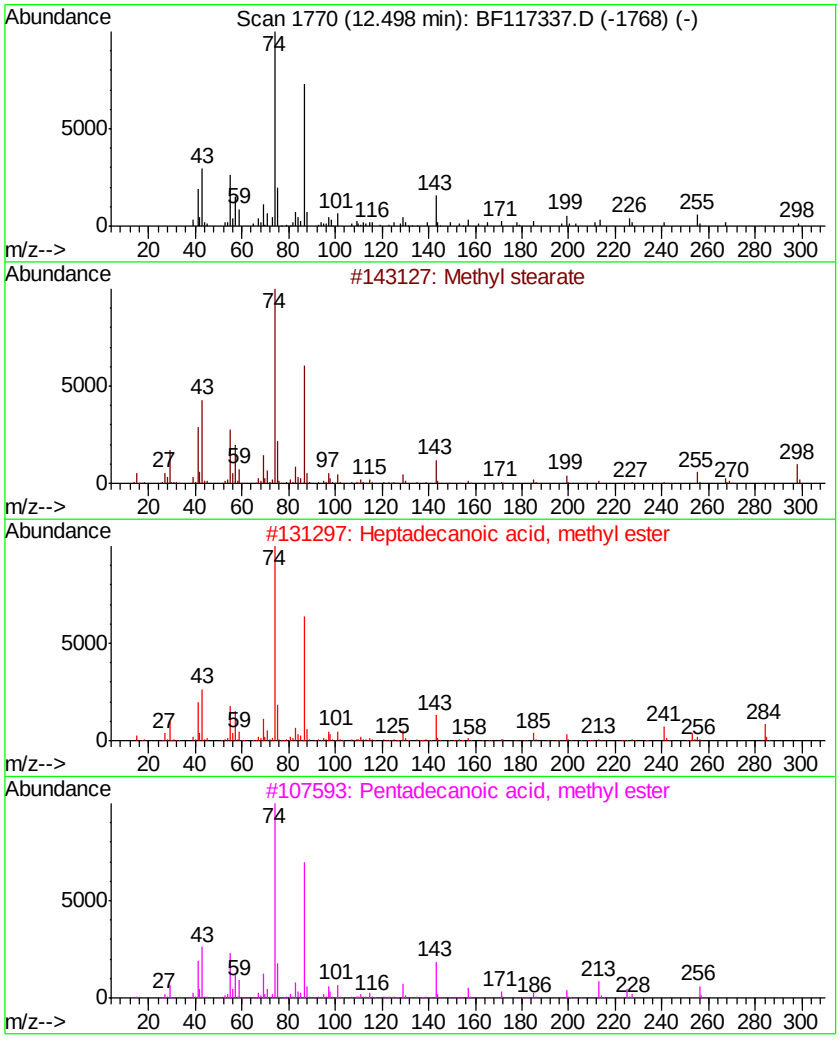
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

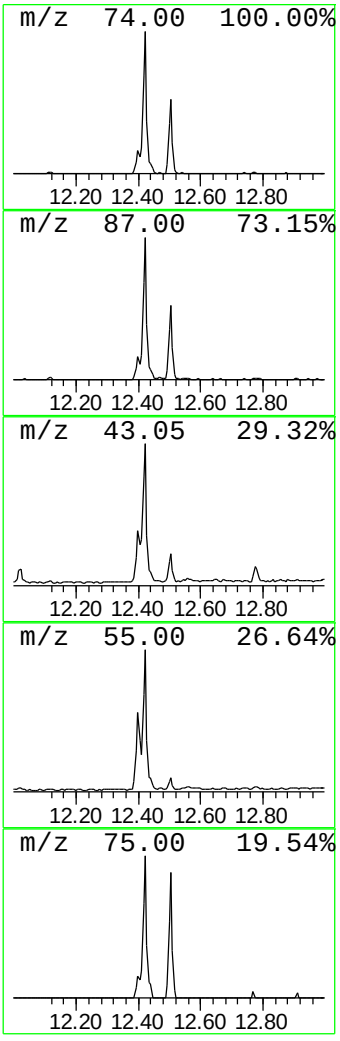
**********

Peak Number 20 Methyl stearate Concentration Rank 17

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.50 | 9.88 ng | 139942 | Phenanthrene-d10 | 11.33 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Methyl stearate | 298 | C19H38O2 | 000112-61-8 | 97 |
| 2 | Heptadecanoic acid, methyl ester | 284 | C18H36O2 | 001731-92-6 | 90 |
| 3 | Pentadecanoic acid, methyl ester | 256 | C16H32O2 | 007132-64-1 | 87 |
| 4 | Methyl tetradecanoate | 242 | C15H30O2 | 000124-10-7 | 86 |
| 5 | Hexadecanoic acid, methyl ester | 270 | C17H34O2 | 000112-39-0 | 86 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100319\
Data File : BF117337.D
Acq On : 4 Oct 2019 00:38
Operator : JU
Sample : K5140-01 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** HR-05-100219

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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 |
| Benzene, 1-ethyl-... | 6.34 | 11.2 | ng | 281167 | 1 | 6.81 | 501568 | 20.0 |
| unknown6.59 | 6.59 | 17.6 | ng | 440848 | 1 | 6.81 | 501568 | 20.0 |
| Decane | 6.65 | 37.8 | ng | 947194 | 1 | 6.81 | 501568 | 20.0 |
| Benzene, 1-ethyl-... | 6.87 | 8.2 | ng | 205811 | 1 | 6.81 | 501568 | 20.0 |
| Benzene, 1-methyl... | 7.09 | 12.8 | ng | 320575 | 1 | 6.81 | 501568 | 20.0 |
| Benzene, 2-ethyl-... | 7.13 | 13.7 | ng | 344466 | 1 | 6.81 | 501568 | 20.0 |
| unknown7.20 | 7.20 | 16.6 | ng | 416836 | 1 | 6.81 | 501568 | 20.0 |
| unknown7.84 | 7.84 | 9.4 | ng | 556955 | 2 | 8.09 | 1183530 | 20.0 |
| Octane, 2,4,6-tri... | 8.68 | 11.6 | ng | 687903 | 2 | 8.09 | 1183530 | 20.0 |
| Octadecane, 1-iodo- | 9.05 | 16.9 | ng | 227681 | 3 | 9.85 | 270302 | 20.0 |
| Dodecane, 2,7,10-... | 9.11 | 21.8 | ng | 294118 | 3 | 9.85 | 270302 | 20.0 |
| Hexadecane | 9.25 | 32.9 | ng | 444762 | 3 | 9.85 | 270302 | 20.0 |
| Naphthalene, 1,2,... | 9.32 | 9.8 | ng | 132848 | 3 | 9.85 | 270302 | 20.0 |
| unknown9.50 | 9.50 | 11.5 | ng | 155578 | 3 | 9.85 | 270302 | 20.0 |
| Decane, 2,3,5-tri... | 9.77 | 13.1 | ng | 177329 | 3 | 9.85 | 270302 | 20.0 |
| Hexadecanoic acid... | 11.72 | 21.8 | ng | 309035 | 4 | 11.33 | 283386 | 20.0 |
| 9,12-Octadecadien... | 12.40 | 74.4 | ng | 1054410 | 4 | 11.33 | 283386 | 20.0 |
| 6-Octadecenoic ac... | 12.42 | 85.8 | ng | 1215030 | 4 | 11.33 | 283386 | 20.0 |
| Methyl stearate | 12.50 | 9.9 | ng | 139942 | 4 | 11.33 | 283386 | 20.0 |