LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
Data File : BF111881.D
Acq On : 7 Jan 2019 17:26
Operator : JU/SJ
Sample : K1053-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

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-BF010719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.199 | 13 | 19 | 29 | rVB | 380964 | 530037 | 10.05% | 0.508% |
| 2 | 2.687 | 96 | 102 | 108 | rBV | 238523 | 386329 | 7.33% | 0.370% |
| 3 | 3.357 | 211 | 216 | 226 | rBV | 96337 | 190606 | 3.61% | 0.183% |
| 4 | 3.981 | 313 | 322 | 325 | rBV | 118762 | 186316 | 3.53% | 0.179% |
| 5 | 4.016 | 325 | 328 | 340 | rVB | 171015 | 313101 | 5.94% | 0.300% |
| 6 | 4.551 | 414 | 419 | 424 | rBV | 310157 | 372007 | 7.06% | 0.357% |
| 7 | 5.116 | 511 | 515 | 519 | rBV2 | 241423 | 514109 | 9.75% | 0.493% |
| 8 | 5.528 | 582 | 585 | 588 | rBV | 1523563 | 1488695 | 28.23% | 1.427% |
| 9 | 5.722 | 604 | 618 | 619 | rBV | 916477 | 2462670 | 46.70% | 2.361% |
| 10 | 5.745 | 619 | 622 | 623 | rVV2 | 357955 | 414444 | 7.86% | 0.397% |
| 11 | 5.787 | 627 | 629 | 631 | rVB | 659265 | 456004 | 8.65% | 0.437% |
| 12 | 5.898 | 639 | 648 | 652 | rBV | 529372 | 1416798 | 26.87% | 1.359% |
| 13 | 5.987 | 661 | 663 | 665 | rVB | 604876 | 422803 | 8.02% | 0.405% |
| 14 | 6.181 | 688 | 696 | 699 | rBV | 1064855 | 1125681 | 21.35% | 1.079% |
| 15 | 6.551 | 753 | 759 | 764 | rBV2 | 1149876 | 1678982 | 31.84% | 1.610% |
| 16 | 6.675 | 775 | 780 | 784 | rBV | 2948535 | 3595776 | 68.19% | 3.448% |
| 17 | 6.728 | 787 | 789 | 791 | rBV2 | 254457 | 251379 | 4.77% | 0.241% |
| 18 | 6.828 | 803 | 806 | 808 | rBV2 | 872104 | 935167 | 17.74% | 0.897% |
| 19 | 6.892 | 814 | 817 | 821 | rBV2 | 1189146 | 1384165 | 26.25% | 1.327% |
| 20 | 6.969 | 828 | 830 | 834 | rVB2 | 4149686 | 5272863 | 100.00% | 5.056% |
| 21 | 7.051 | 840 | 844 | 848 | rBV3 | 3575133 | 4048978 | 76.79% | 3.882% |
| 22 | 7.092 | 848 | 851 | 854 | rVB | 305144 | 307659 | 5.83% | 0.295% |
| 23 | 7.151 | 856 | 861 | 867 | rVB3 | 659259 | 1051198 | 19.94% | 1.008% |
| 24 | 7.216 | 867 | 872 | 876 | rBV4 | 202410 | 329888 | 6.26% | 0.316% |
| 25 | 7.310 | 880 | 888 | 891 | rBV | 2234772 | 2805510 | 53.21% | 2.690% |
| 26 | 7.410 | 891 | 905 | 907 | rVV | 923324 | 2766370 | 52.46% | 2.653% |
| 27 | 7.451 | 907 | 912 | 915 | rVV | 2283101 | 2303911 | 43.69% | 2.209% |
| 28 | 7.498 | 915 | 920 | 925 | rVB2 | 146201 | 220647 | 4.18% | 0.212% |
| 29 | 7.639 | 937 | 944 | 946 | rBV2 | 576364 | 939377 | 17.82% | 0.901% |
| 30 | 7.734 | 950 | 960 | 961 | rVB | 1313039 | 3163976 | 60.00% | 3.034% |
| 31 | 7.769 | 964 | 966 | 967 | rBV | 323366 | 191366 | 3.63% | 0.183% |
| 32 | 7.792 | 967 | 970 | 973 | rVB3 | 214153 | 295974 | 5.61% | 0.284% |
| 33 | 7.834 | 973 | 977 | 983 | rVB | 1859894 | 2466664 | 46.78% | 2.365% |
| 34 | 7.957 | 992 | 998 | 999 | rBV | 2141496 | 2877608 | 54.57% | 2.759% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
Data File : BF111881.D
Acq On : 7 Jan 2019 17:26
Operator : JU/SJ
Sample : K1053-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

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-BF010719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 7.975 | 999 | 1001 | 1004 | rVB2 | 1231895 | 984949 | 18.68% | 0.944% |
| 36 | 8.016 | 1004 | 1008 | 1009 | rBV | 755239 | 849449 | 16.11% | 0.815% |
| 37 | 8.034 | 1009 | 1011 | 1013 | rBV2 | 460829 | 429575 | 8.15% | 0.412% |
| 38 | 8.104 | 1020 | 1023 | 1025 | rBV | 1034846 | 1229660 | 23.32% | 1.179% |
| 39 | 8.210 | 1039 | 1041 | 1043 | rVB | 2208737 | 1431753 | 27.15% | 1.373% |
| 40 | 8.281 | 1044 | 1053 | 1054 | rBV2 | 1198377 | 1891579 | 35.87% | 1.814% |
| 41 | 8.310 | 1055 | 1058 | 1061 | rVV2 | 2403966 | 2989288 | 56.69% | 2.866% |
| 42 | 8.345 | 1061 | 1064 | 1068 | rVB | 1283911 | 1223128 | 23.20% | 1.173% |
| 43 | 8.381 | 1068 | 1070 | 1072 | rVB | 314912 | 230779 | 4.38% | 0.221% |
| 44 | 8.416 | 1072 | 1076 | 1079 | rBV | 1206816 | 1081153 | 20.50% | 1.037% |
| 45 | 8.451 | 1079 | 1082 | 1086 | rVB | 689135 | 704729 | 13.37% | 0.676% |
| 46 | 8.498 | 1086 | 1090 | 1092 | rBV | 657228 | 751049 | 14.24% | 0.720% |
| 47 | 8.539 | 1092 | 1097 | 1100 | rVV2 | 3714102 | 4281399 | 81.20% | 4.105% |
| 48 | 8.575 | 1100 | 1103 | 1104 | rVV2 | 577446 | 596382 | 11.31% | 0.572% |
| 49 | 8.604 | 1104 | 1108 | 1112 | rVV2 | 570205 | 979763 | 18.58% | 0.939% |
| 50 | 8.639 | 1112 | 1114 | 1119 | rVV3 | 1127798 | 1504872 | 28.54% | 1.443% |
| 51 | 8.698 | 1119 | 1124 | 1125 | rVV | 360325 | 461291 | 8.75% | 0.442% |
| 52 | 8.710 | 1125 | 1126 | 1129 | rVB2 | 304455 | 192675 | 3.65% | 0.185% |
| 53 | 8.751 | 1129 | 1133 | 1135 | rBV | 772151 | 965365 | 18.31% | 0.926% |
| 54 | 8.775 | 1135 | 1137 | 1139 | rVB | 1051585 | 729640 | 13.84% | 0.700% |
| 55 | 8.845 | 1143 | 1149 | 1150 | rBV5 | 363018 | 573953 | 10.89% | 0.550% |
| 56 | 8.863 | 1150 | 1152 | 1154 | rVV3 | 607985 | 489735 | 9.29% | 0.470% |
| 57 | 8.916 | 1158 | 1161 | 1163 | rVV2 | 265235 | 296136 | 5.62% | 0.284% |
| 58 | 8.939 | 1163 | 1165 | 1171 | rVB2 | 1606458 | 1644132 | 31.18% | 1.577% |
| 59 | 8.986 | 1171 | 1173 | 1178 | rVB3 | 333185 | 339652 | 6.44% | 0.326% |
| 60 | 9.033 | 1178 | 1181 | 1183 | rBV | 427391 | 413953 | 7.85% | 0.397% |
| 61 | 9.057 | 1183 | 1185 | 1186 | rVV | 912493 | 875789 | 16.61% | 0.840% |
| 62 | 9.069 | 1186 | 1187 | 1194 | rVB | 1678901 | 1526571 | 28.95% | 1.464% |
| 63 | 9.128 | 1194 | 1197 | 1199 | rBV | 1004562 | 909888 | 17.26% | 0.872% |
| 64 | 9.163 | 1199 | 1203 | 1207 | rVB3 | 863772 | 1149583 | 21.80% | 1.102% |
| 65 | 9.204 | 1207 | 1210 | 1213 | rBV | 410300 | 394398 | 7.48% | 0.378% |
| 66 | 9.251 | 1213 | 1218 | 1221 | rBV | 4473221 | 4488850 | 85.13% | 4.304% |
| 67 | 9.310 | 1225 | 1228 | 1230 | rBV2 | 332725 | 339039 | 6.43% | 0.325% |
| 68 | 9.339 | 1230 | 1233 | 1237 | rVV | 802134 | 1014431 | 19.24% | 0.973% |
| 69 | 9.416 | 1241 | 1246 | 1250 | rBV2 | 396880 | 406765 | 7.71% | 0.390% |
| 70 | 9.463 | 1250 | 1254 | 1257 | rVB4 | 132810 | 170975 | 3.24% | 0.164% |
| 71 | 9.504 | 1257 | 1261 | 1264 | rBV2 | 577671 | 828680 | 15.72% | 0.795% |

LSC Area Percent Report

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Acq On : 7 Jan 2019 17:26
Operator : JU/SJ
Sample : K1053-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

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-BF010719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 72 | 9.533 | 1264 | 1266 | 1268 | rVV2 | 586413 | 570462 | 10.82% | 0.547% |
| 73 | 9.557 | 1268 | 1270 | 1274 | rVV2 | 407605 | 450127 | 8.54% | 0.432% |
| 74 | 9.604 | 1274 | 1278 | 1281 | rVB2 | 166654 | 227212 | 4.31% | 0.218% |
| 75 | 9.639 | 1281 | 1284 | 1287 | rBV3 | 101902 | 179227 | 3.40% | 0.172% |
| 76 | 9.675 | 1287 | 1290 | 1293 | rVV3 | 796366 | 978028 | 18.55% | 0.938% |
| 77 | 9.704 | 1293 | 1295 | 1299 | rVV2 | 484133 | 761975 | 14.45% | 0.731% |
| 78 | 9.745 | 1299 | 1302 | 1306 | rVV3 | 475080 | 778335 | 14.76% | 0.746% |
| 79 | 9.792 | 1309 | 1310 | 1313 | rVV | 407742 | 322277 | 6.11% | 0.309% |
| 80 | 9.839 | 1316 | 1318 | 1319 | rVV | 228784 | 181115 | 3.43% | 0.174% |
| 81 | 9.857 | 1319 | 1321 | 1326 | rVV3 | 224680 | 220579 | 4.18% | 0.212% |
| 82 | 9.928 | 1330 | 1333 | 1336 | rVB2 | 1256202 | 1126466 | 21.36% | 1.080% |
| 83 | 9.992 | 1340 | 1344 | 1347 | rBV2 | 158458 | 264937 | 5.02% | 0.254% |
| 84 | 10.069 | 1354 | 1357 | 1360 | rBV2 | 215666 | 280214 | 5.31% | 0.269% |
| 85 | 10.098 | 1360 | 1362 | 1367 | rVB5 | 211632 | 265961 | 5.04% | 0.255% |
| 86 | 10.357 | 1401 | 1406 | 1409 | rVB3 | 190161 | 306022 | 5.80% | 0.293% |
| 87 | 10.463 | 1421 | 1424 | 1431 | rVB3 | 367753 | 472980 | 8.97% | 0.454% |
| 88 | 10.722 | 1464 | 1468 | 1471 | rBV | 2649054 | 2334871 | 44.28% | 2.239% |
| 89 | 11.004 | 1511 | 1516 | 1520 | rVV | 430663 | 517649 | 9.82% | 0.496% |
| 90 | 11.198 | 1546 | 1549 | 1552 | rVB | 219321 | 192744 | 3.66% | 0.185% |
| 91 | 11.416 | 1582 | 1586 | 1591 | rVB | 1039131 | 971072 | 18.42% | 0.931% |
| 92 | 11.939 | 1672 | 1675 | 1678 | rBV | 391584 | 337023 | 6.39% | 0.323% |
| 93 | 12.380 | 1747 | 1750 | 1757 | rBV3 | 144034 | 196486 | 3.73% | 0.188% |
| 94 | 12.674 | 1798 | 1800 | 1804 | rBV | 268447 | 223539 | 4.24% | 0.214% |
| 95 | 12.727 | 1805 | 1809 | 1811 | rVV | 281303 | 269054 | 5.10% | 0.258% |
| 96 | 12.998 | 1851 | 1855 | 1858 | rVB | 3256238 | 2960754 | 56.15% | 2.839% |
| 97 | 13.868 | 2001 | 2003 | 2010 | rBV5 | 97673 | 170849 | 3.24% | 0.164% |
| 98 | 14.051 | 2030 | 2034 | 2040 | rVB | 1036484 | 879381 | 16.68% | 0.843% |
| 99 | 14.863 | 2169 | 2172 | 2176 | rVB | 286740 | 279409 | 5.30% | 0.268% |
| 100 | 15.533 | 2281 | 2286 | 2295 | rVB | 793375 | 1032680 | 19.58% | 0.990% |

Sum of corrected areas: 104289494

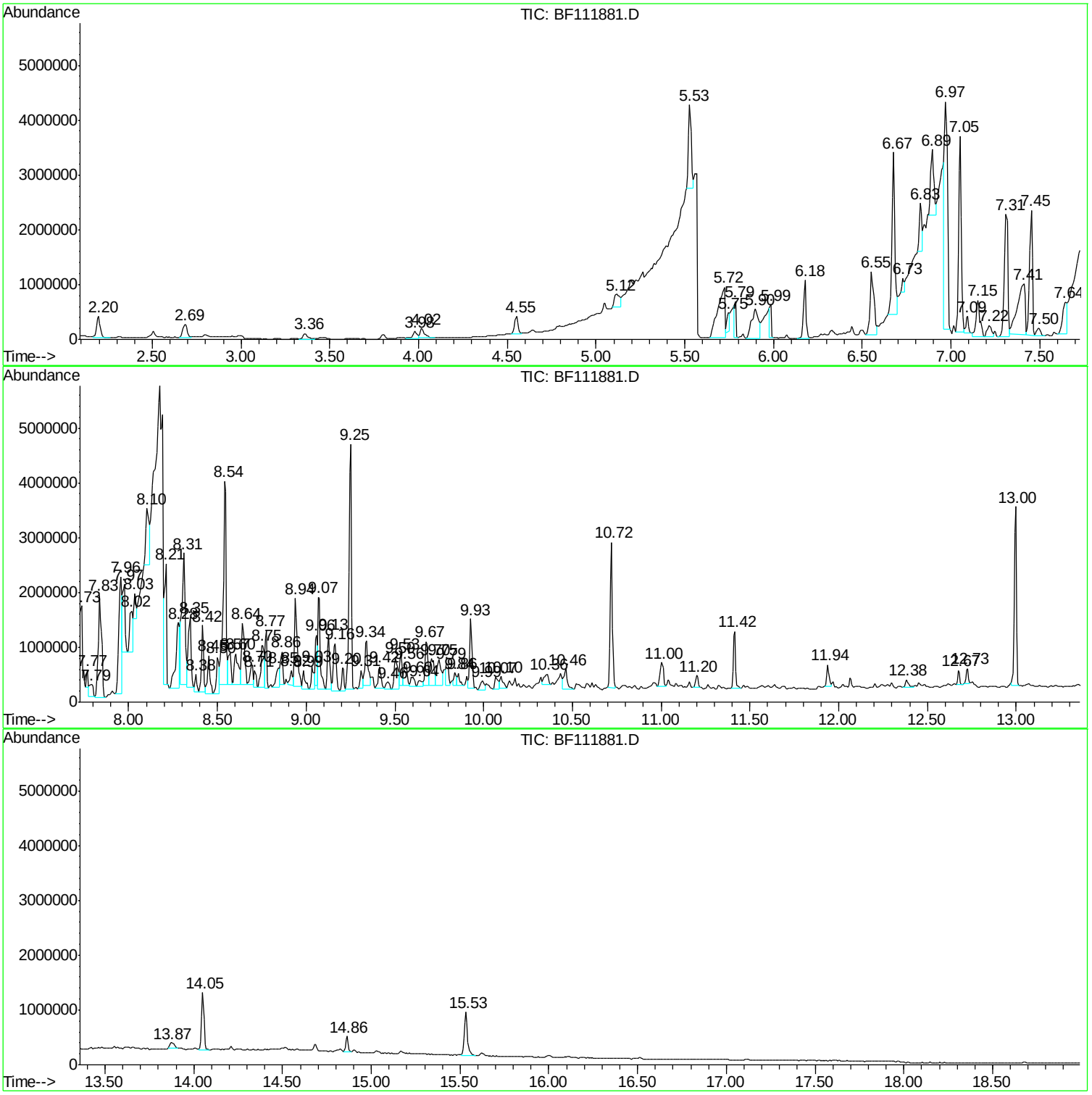
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
Data File : BF111881.D
Acq On : 7 Jan 2019 17:26
Operator : JU/SJ
Sample : K1053-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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\BF010719\
Data File : BF111881.D
Acq On : 7 Jan 2019 17:26
Operator : JU/SJ
Sample : K1053-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

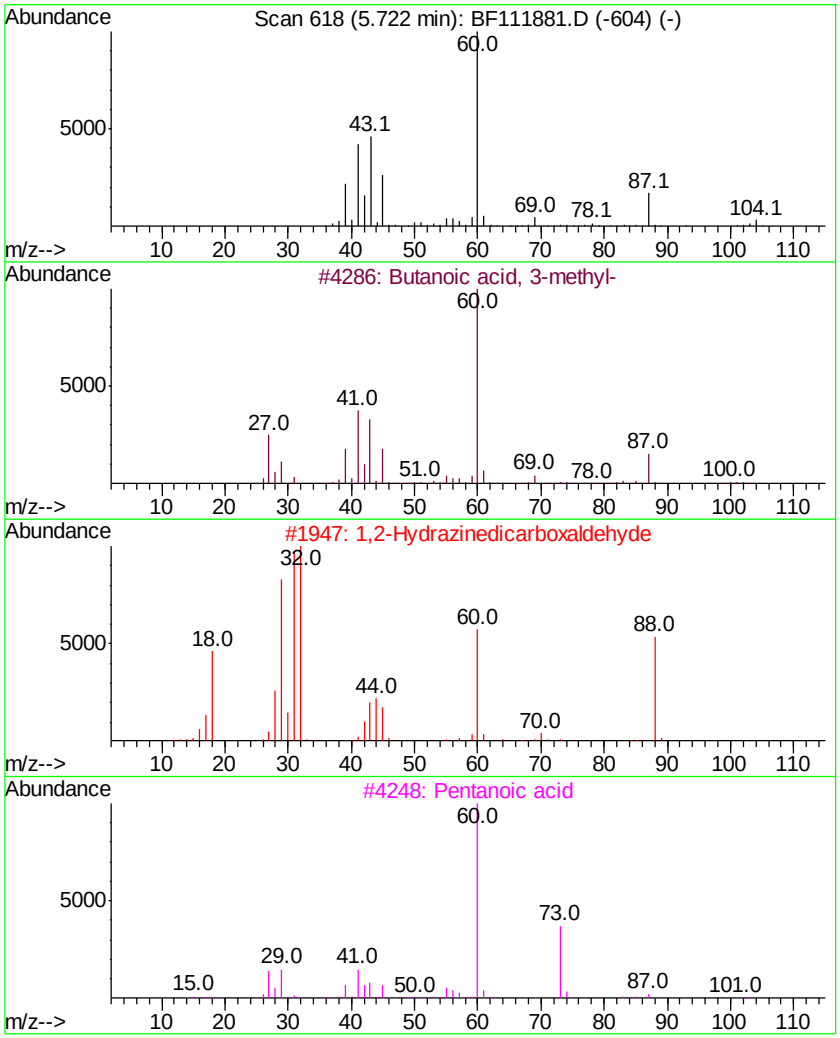
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

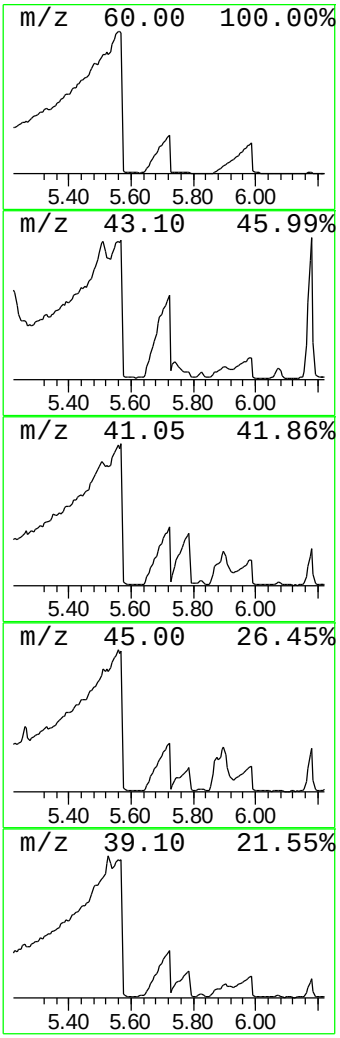
**********

Peak Number 1 Butanoic acid, 3-methyl- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.72 | 35.58 ng | 2462670 | 1,4-Dichlorobenzene-d4 | 6.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butanoic acid, 3-methyl- | 102 | C5H10O2 | 000503-74-2 | 90 |
| 2 | 1,2-Hydrazinedicarboxaldehyde | 88 | C2H4N2O2 | 000628-36-4 | 39 |
| 3 | Pentanoic acid | 102 | C5H10O2 | 000109-52-4 | 36 |
| 4 | 1-Pentanamine | 87 | C5H13N | 000110-58-7 | 9 |
| 5 | Formic acid hydrazide | 60 | CH4N2O | 000624-84-0 | 9 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
Data File : BF111881.D
Acq On : 7 Jan 2019 17:26
Operator : JU/SJ
Sample : K1053-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

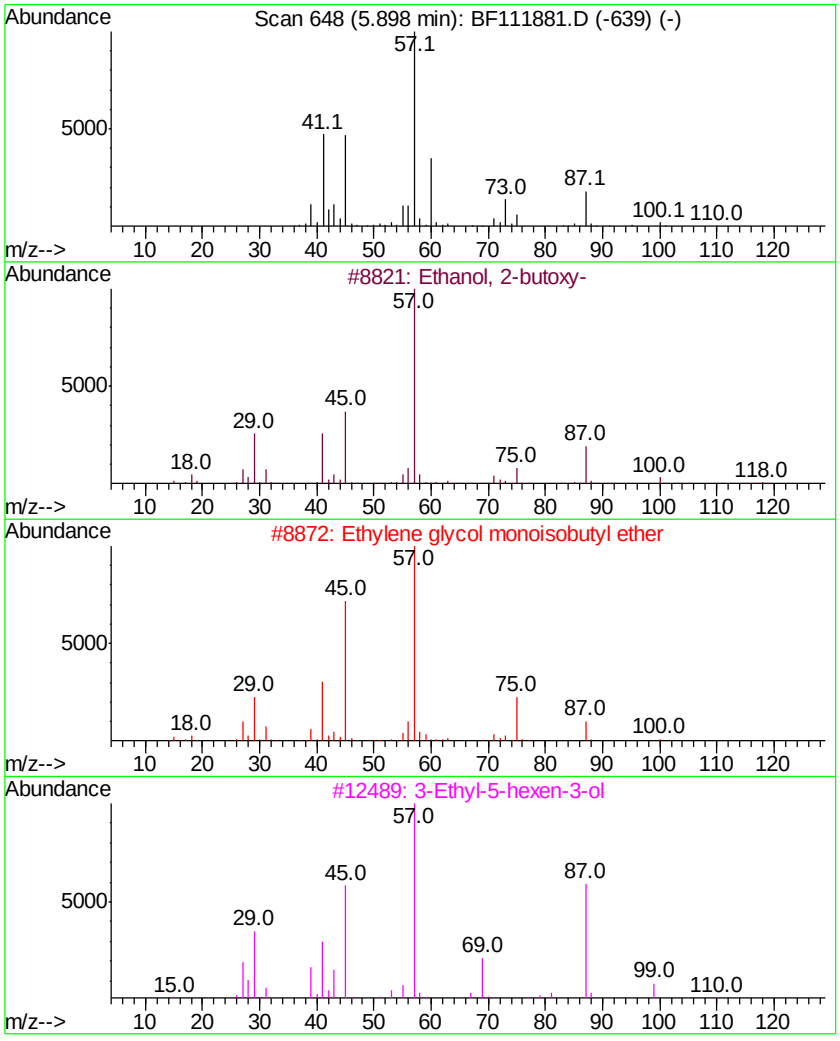
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

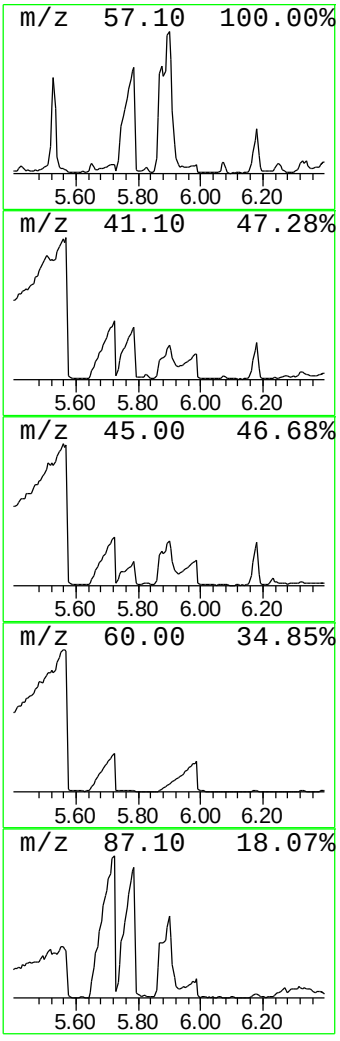
**********

Peak Number 2 Ethanol, 2-butoxy- Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.90 | 20.47 ng | 1416800 | 1,4-Dichlorobenzene-d4 | 6.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2-butoxy- | 118 | C6H14O2 | 000111-76-2 | 53 |
| 2 | Ethylene glycol monoisobutyl ether | 118 | C6H14O2 | 004439-24-1 | 40 |
| 3 | 3-Ethyl-5-hexen-3-ol | 128 | C8H16O | 001907-46-6 | 38 |
| 4 | 3,3-Dimethylbutane-2-ol | 102 | C6H14O | 000464-07-3 | 37 |
| 5 | Butoxyacetic acid | 132 | C6H12O3 | 002516-93-0 | 25 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
Data File : BF111881.D
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Sample : K1053-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

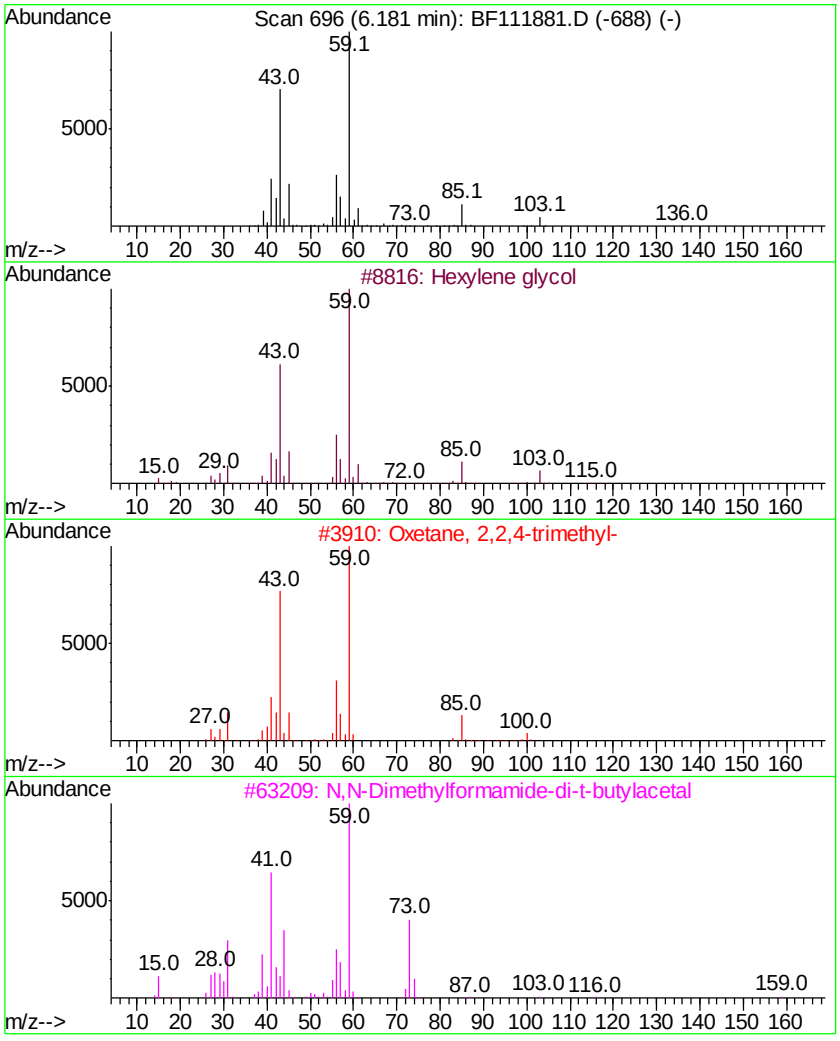
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

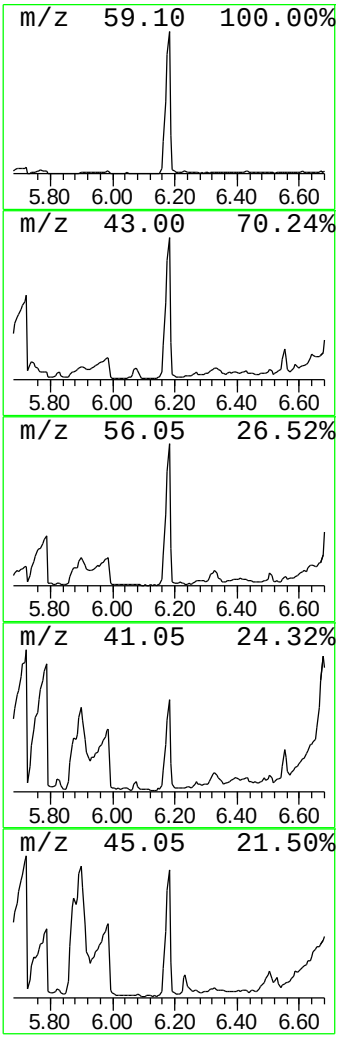
**********

Peak Number 3 Hexylene glycol Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.18 | 16.27 ng | 1125680 | 1,4-Dichlorobenzene-d4 | 6.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexylene glycol | 118 | C6H14O2 | 000107-41-5 | 90 |
| 2 | Oxetane, 2,2,4-trimethyl- | 100 | C6H12O | 023120-44-7 | 72 |
| 3 | N,N-Dimethylformamide-di-t-butyl... | 203 | C11H25NO2 | 036805-97-7 | 45 |
| 4 | dl-Erythro-O-methylthreonine | 133 | C5H11NO3 | 1000214-70-7 | 45 |
| 5 | 2-Butanol, 3-methoxy- | 104 | C5H12O2 | 053778-72-6 | 40 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
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**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

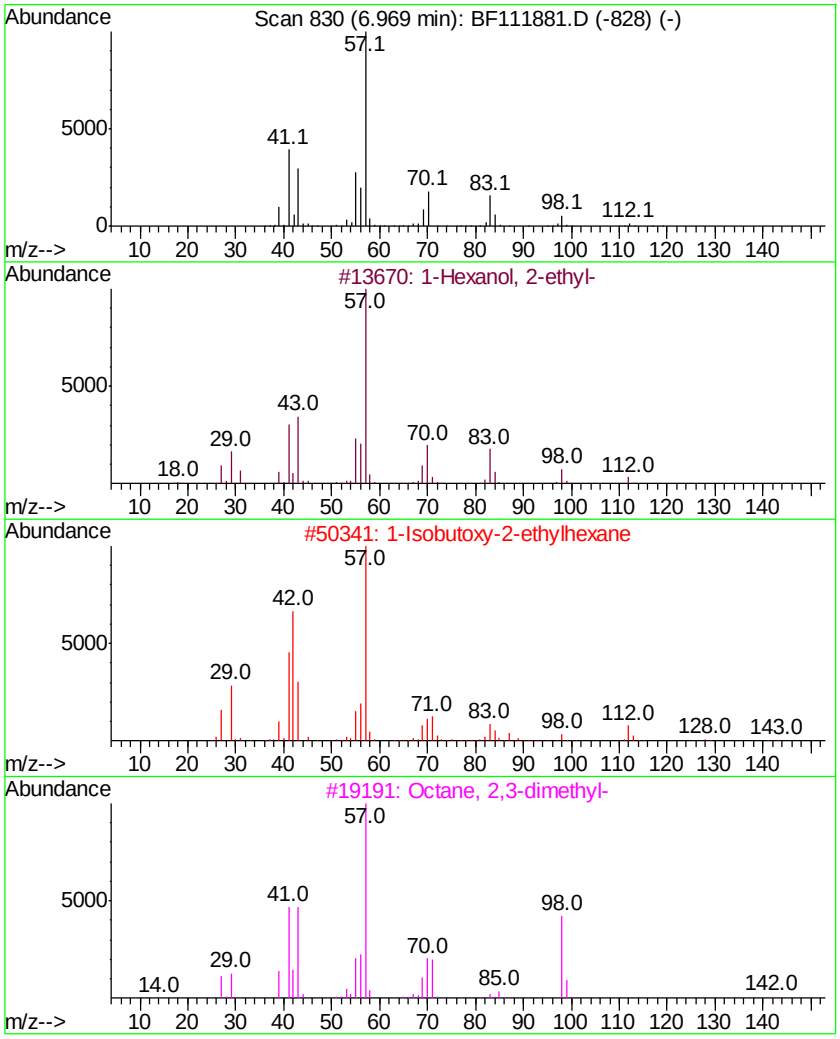
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

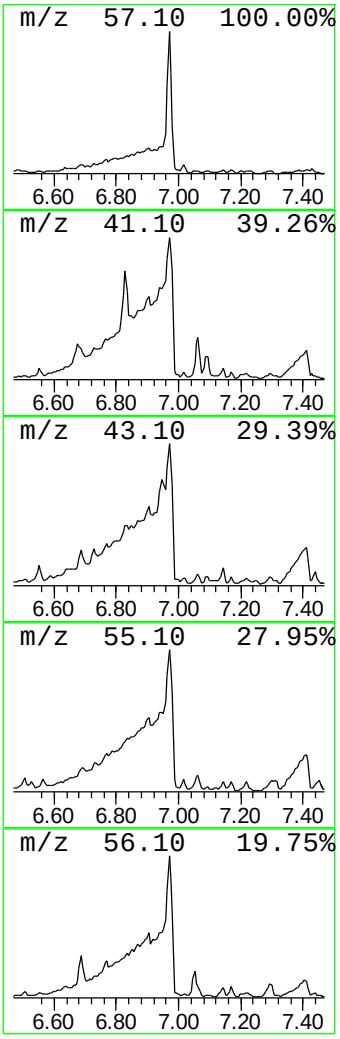
**********

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.97 | 76.19 ng | 5272860 | 1,4-Dichlorobenzene-d4 | 6.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Hexanol, 2-ethyl- | 130 | C8H18O | 000104-76-7 | 83 |
| 2 | 1-Isobutoxy-2-ethylhexane | 186 | C12H26O | 1000139-90-3 | 56 |
| 3 | Octane, 2,3-dimethyl- | 142 | C10H22 | 007146-60-3 | 50 |
| 4 | 1-Pentanol, 2-ethyl-4-methyl- | 130 | C8H18O | 000106-67-2 | 45 |
| 5 | 1-Pentene, 2,4,4-trimethyl- | 112 | C8H16 | 000107-39-1 | 43 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
Data File : BF111881.D
Acq On : 7 Jan 2019 17:26
Operator : JU/SJ
Sample : K1053-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

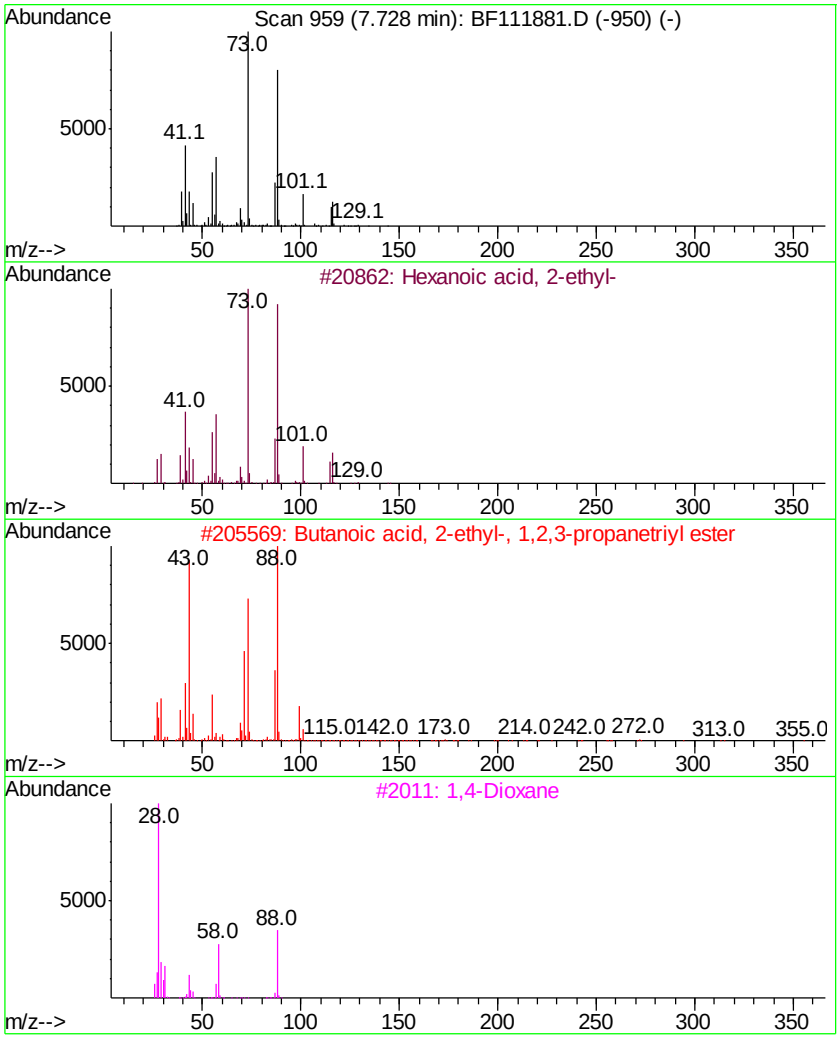
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

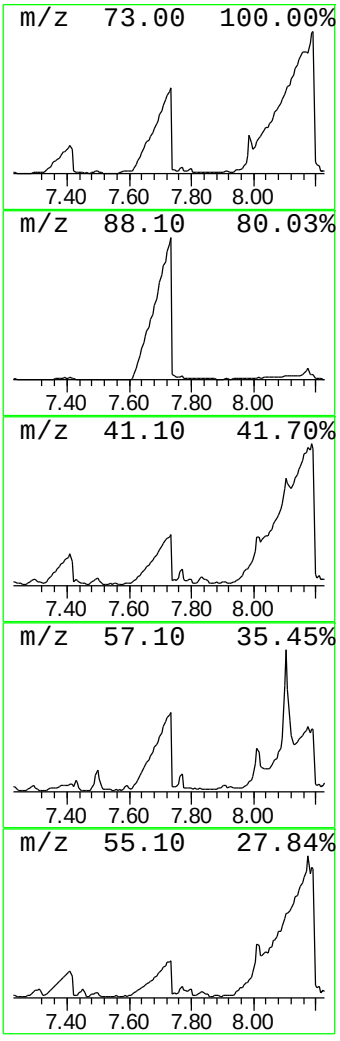
**********

Peak Number 6 Hexanoic acid, 2-ethyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.73 | 44.20 ng | 3163980 | Naphthalene-d8 | 8.17 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexanoic acid, 2-ethyl- | 144 | C8H16O2 | 000149-57-5 | 86 |
| 2 | Butanoic acid, 2-ethyl-, 1,2,3-p... | 386 | C21H38O6 | 056554-54-2 | 42 |
| 3 | 1,4-Dioxane | 88 | C4H8O2 | 000123-91-1 | 37 |
| 4 | Pentanoic acid, 2,4-dimethyl-, m... | 144 | C8H16O2 | 071672-33-8 | 37 |
| 5 | L(-)-Fucose, tetramethyl ether | 220 | C10H20O5 | 1000332-75-0 | 28 |



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Data File : BF111881.D
Acq On : 7 Jan 2019 17:26
Operator : JU/SJ
Sample : K1053-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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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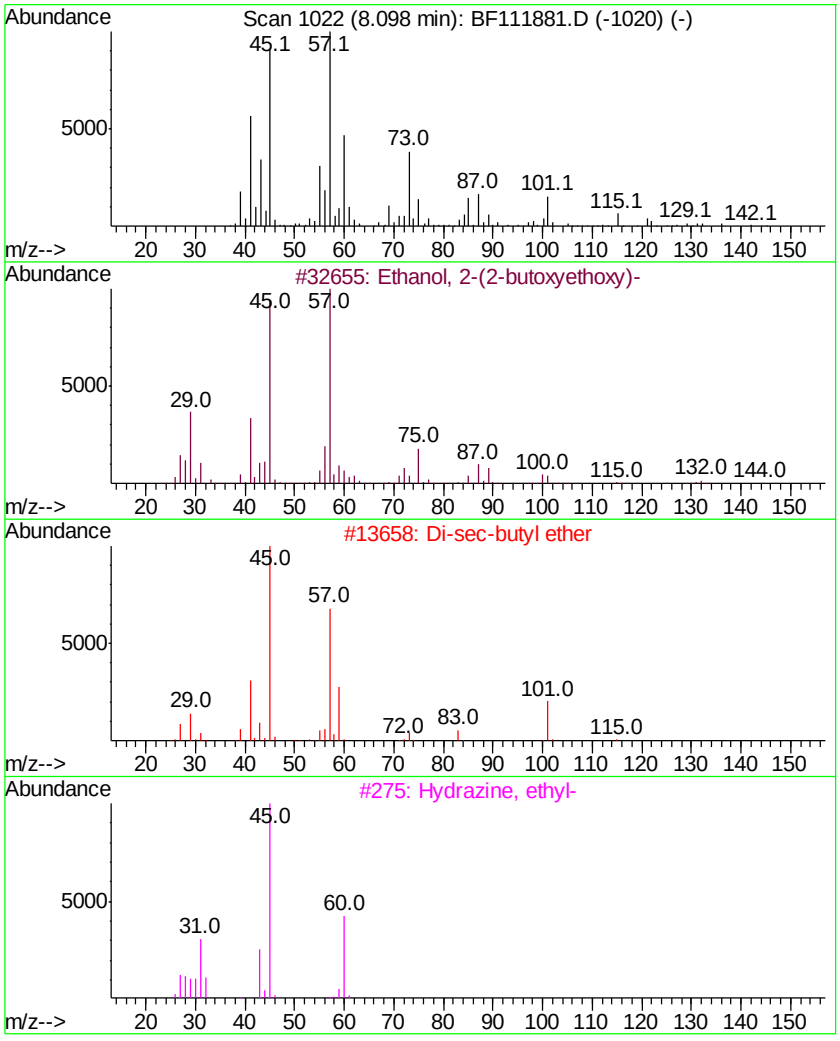
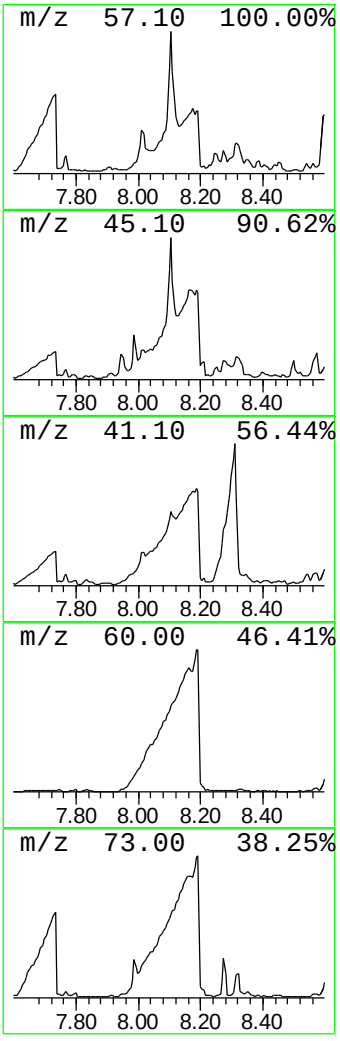
Peak Number 7 unknown8.10 Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.10 | 17.18 ng | 1229660 | Naphthalene-d8 | 8.17 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2-(2-butoxyethoxy)- | 162 | C8H18O3 | 000112-34-5 | 47 |
| 2 | Di-sec-butyl ether | 130 | C8H18O | 006863-58-7 | 43 |
| 3 | Hydrazine, ethyl- | 60 | C2H8N2 | 000624-80-6 | 43 |
| 4 | Propane, 2-ethoxy- | 88 | C5H12O | 000625-54-7 | 38 |
| 5 | Methoxyacetic acid, heptyl ester | 188 | C10H20O3 | 168920-36-3 | 38 |



Library Search Compound Report

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Data File : BF111881.D
Acq On : 7 Jan 2019 17:26
Operator : JU/SJ
Sample : K1053-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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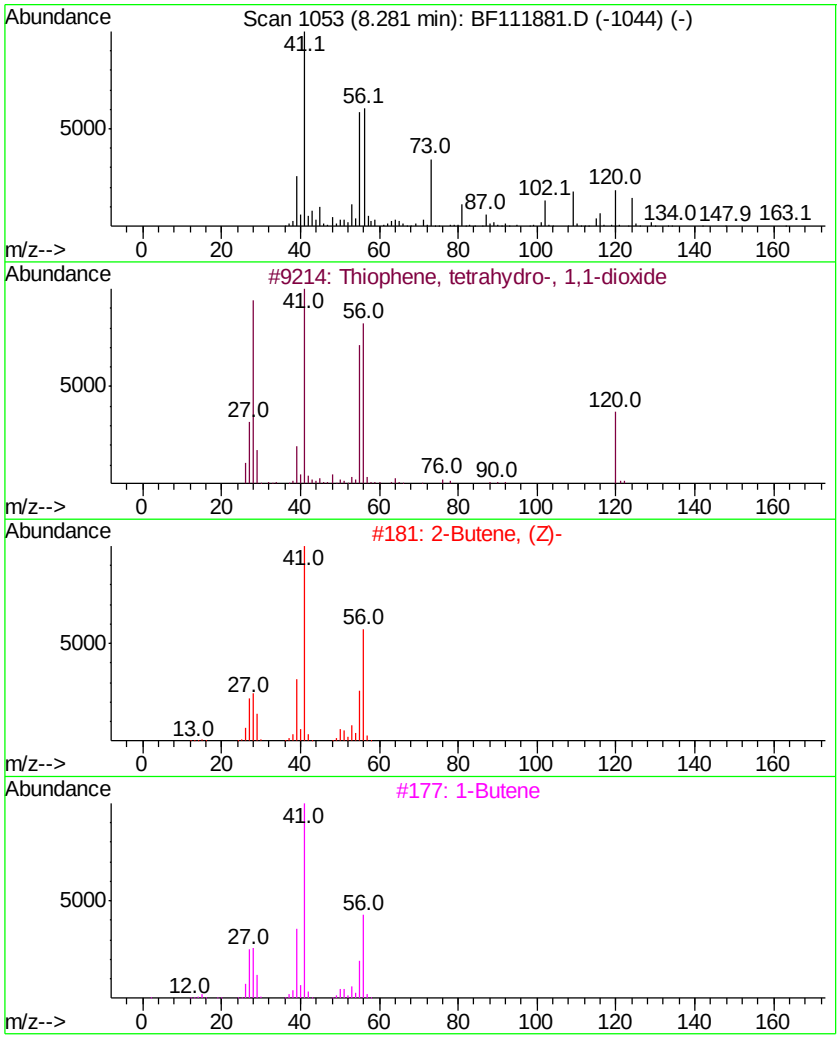
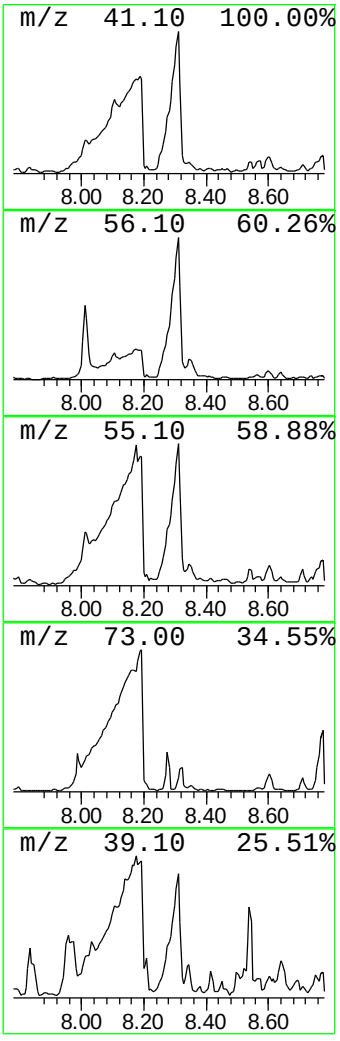
Peak Number 8 unknown8.28 Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.28 | 26.42 ng | 1891580 | Naphthalene-d8 | 8.17 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Thiophene, tetrahydro-, 1,1-dioxide | 120 | C4H8O2S | 000126-33-0 | 30 |
| 2 | 2-Butene, (Z)- | 56 | C4H8 | 000590-18-1 | 18 |
| 3 | 1-Butene | 56 | C4H8 | 000106-98-9 | 14 |
| 4 | 2-Butene, (E)- | 56 | C4H8 | 000624-64-6 | 14 |
| 5 | Cyclobutane | 56 | C4H8 | 000287-23-0 | 14 |



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Acq On : 7 Jan 2019 17:26
Operator : JU/SJ
Sample : K1053-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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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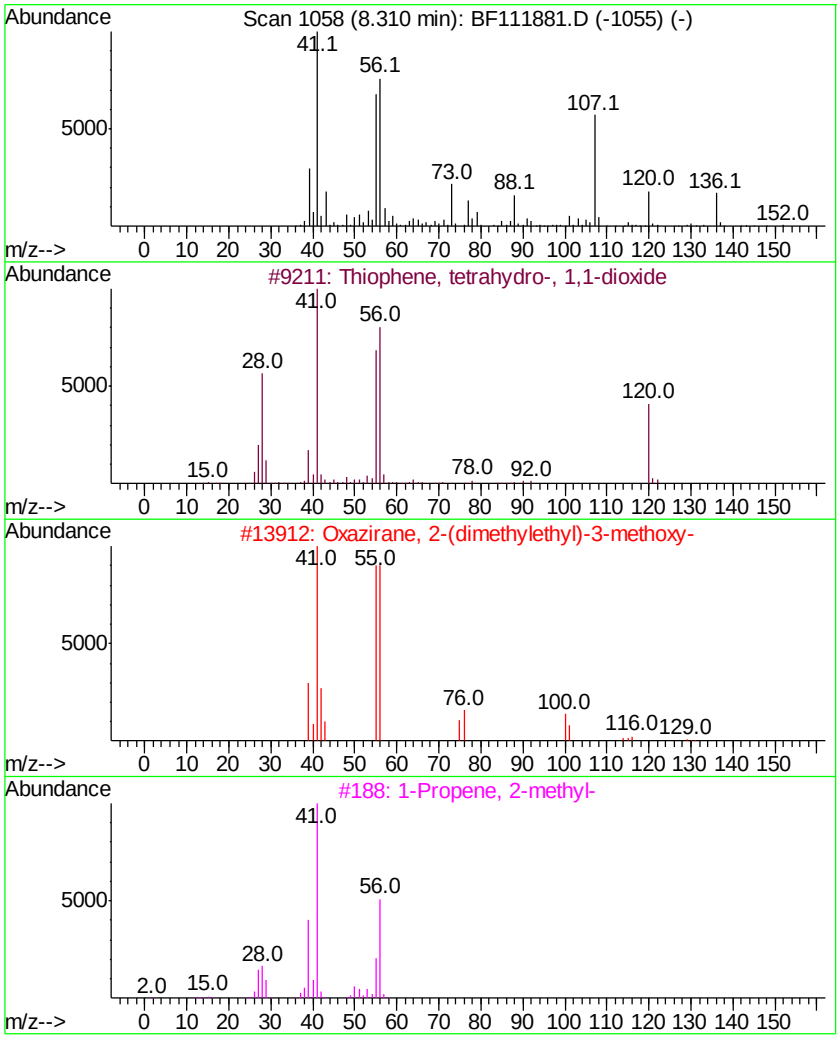
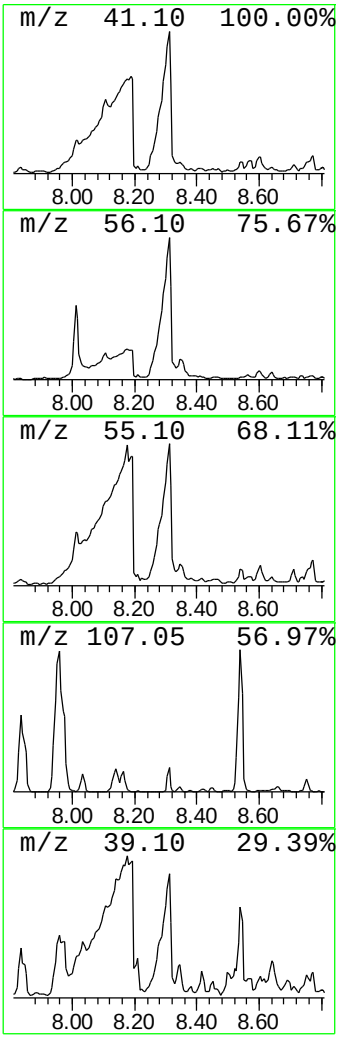
Peak Number 9 unknown8.31 Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.31 | 41.76 ng | 2989290 | Naphthalene-d8 | 8.17 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Thiophene, tetrahydro-, 1,1-dioxide | 120 | C4H8O2S | 000126-33-0 | 38 |
| 2 | Oxazirane, 2-(dimethylethyl)-3-m... | 131 | C6H13NO2 | 103202-91-1 | 35 |
| 3 | 1-Propene, 2-methyl- | 56 | C4H8 | 000115-11-7 | 27 |
| 4 | 4-Penten-2-ol, 3-methyl- | 100 | C6H12O | 001569-59-1 | 27 |
| 5 | Oxetane, 2,3,4-trimethyl-, (2.al... | 100 | C6H12O | 032347-12-9 | 27 |



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Data File : BF111881.D
Acq On : 7 Jan 2019 17:26
Operator : JU/SJ
Sample : K1053-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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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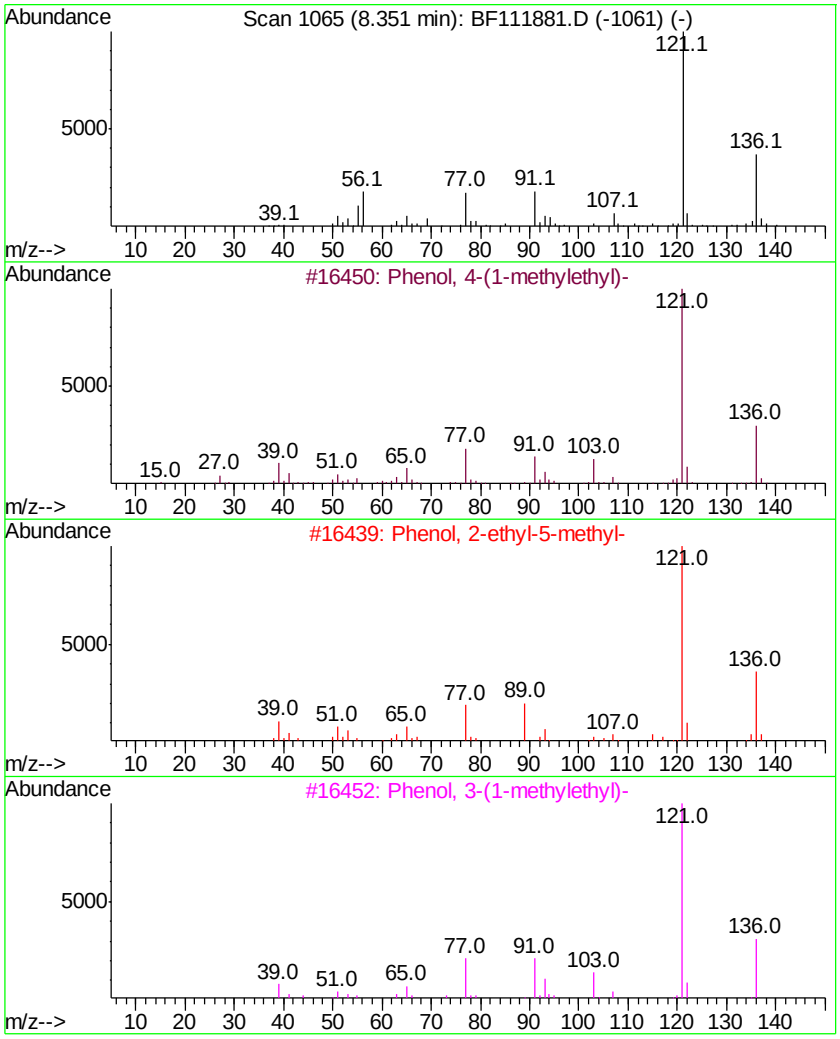
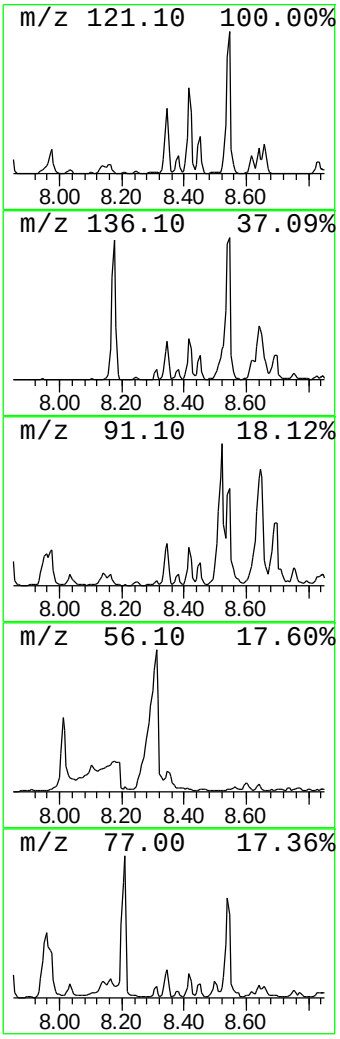
Peak Number 10 Phenol, 4-(1-methylethyl)- Concentration Rank 15

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.35 | 17.09 ng | 1223130 | Naphthalene-d8 | 8.17 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenol, 4-(1-methylethyl)- | 136 | C9H12O | 000099-89-8 | 91 |
| 2 | Phenol, 2-ethyl-5-methyl- | 136 | C9H12O | 001687-61-2 | 87 |
| 3 | Phenol, 3-(1-methylethyl)- | 136 | C9H12O | 000618-45-1 | 87 |
| 4 | Phenol, 2,4,6-trimethyl- | 136 | C9H12O | 000527-60-6 | 86 |
| 5 | Phenol, 2-ethyl-6-methyl- | 136 | C9H12O | 001687-64-5 | 83 |



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Acq On : 7 Jan 2019 17:26
Operator : JU/SJ
Sample : K1053-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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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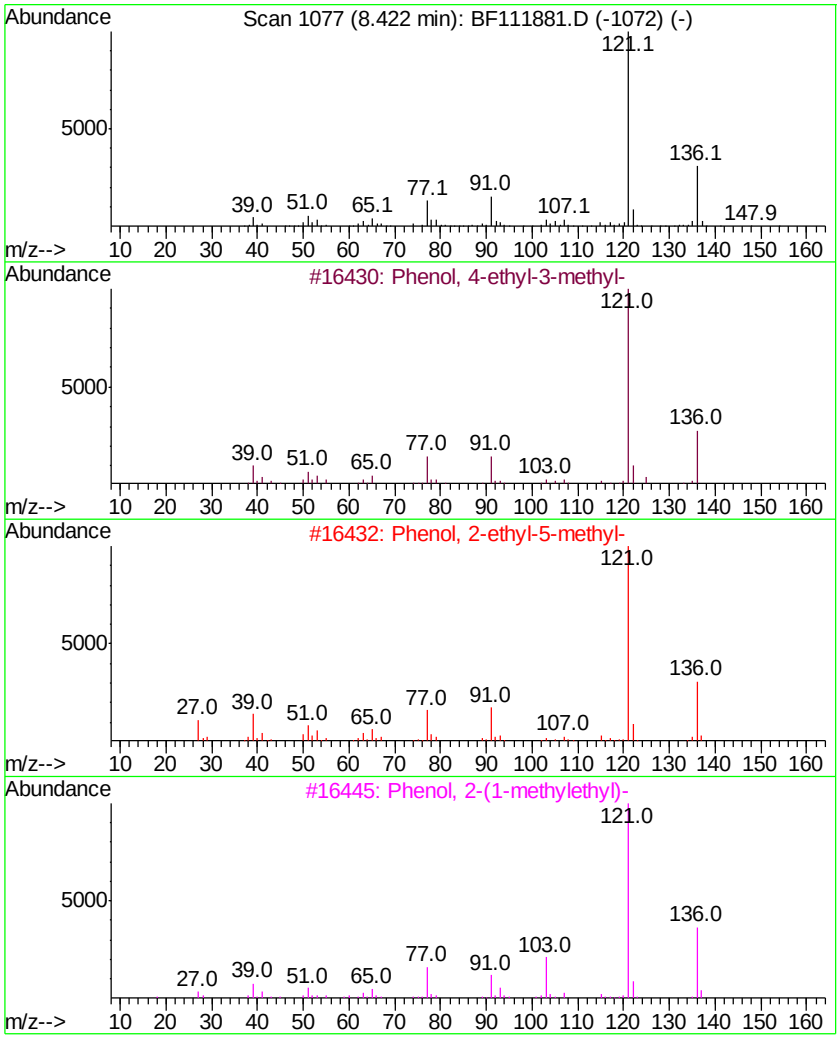
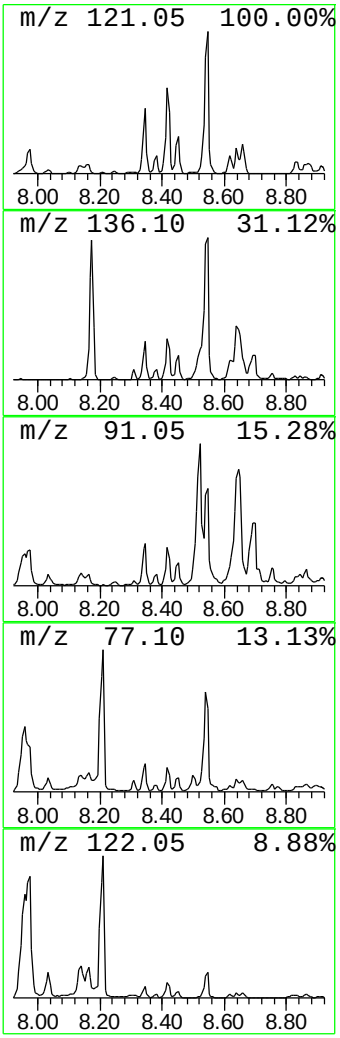
Peak Number 11 Phenol, 4-ethyl-3-methyl- Concentration Rank 19

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.42 | 15.10 ng | 1081150 | Naphthalene-d8 | 8.17 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenol, 4-ethyl-3-methyl- | 136 | C9H12O | 001123-94-0 | 95 |
| 2 | Phenol, 2-ethyl-5-methyl- | 136 | C9H12O | 001687-61-2 | 91 |
| 3 | Phenol, 2-(1-methylethyl)- | 136 | C9H12O | 000088-69-7 | 91 |
| 4 | Phenol, 3-ethyl-5-methyl- | 136 | C9H12O | 000698-71-5 | 90 |
| 5 | Benzene, 1-ethyl-4-methoxy- | 136 | C9H12O | 001515-95-3 | 87 |



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Acq On : 7 Jan 2019 17:26
Operator : JU/SJ
Sample : K1053-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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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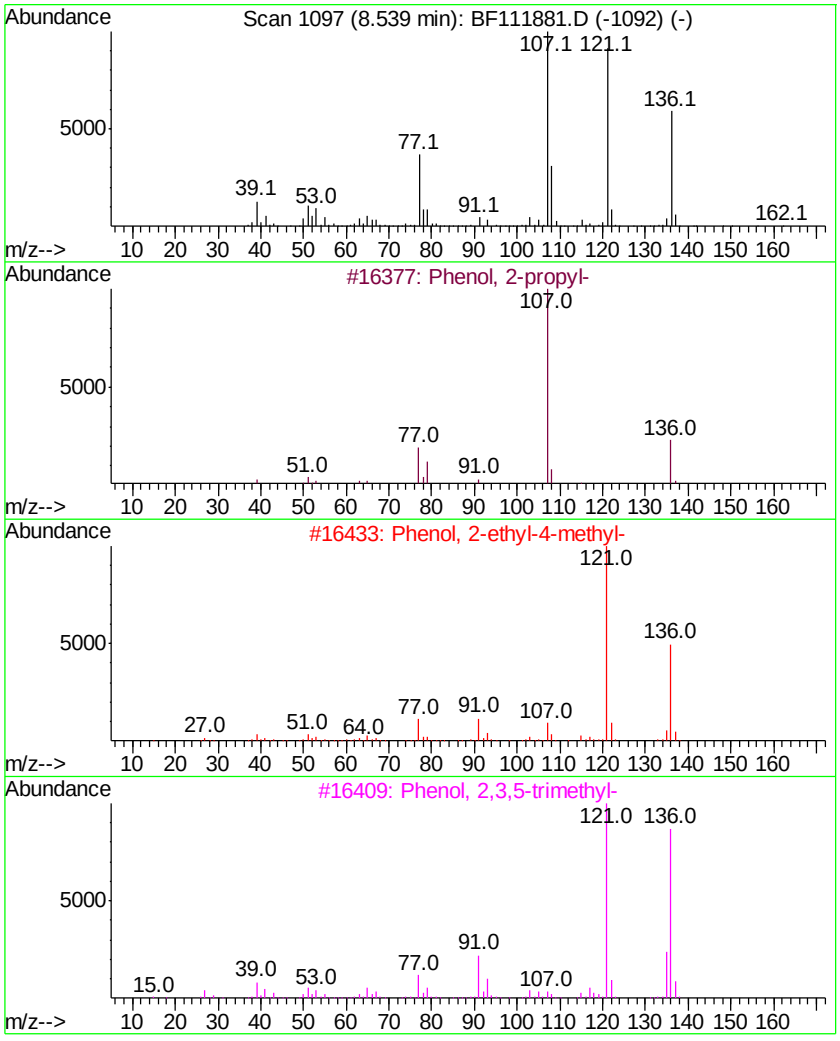
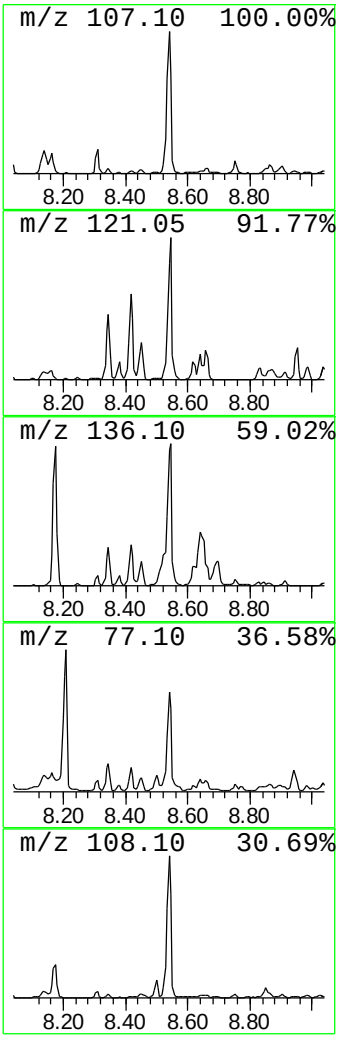
Peak Number 12 unknown8.54 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.54 | 59.81 ng | 4281400 | Naphthalene-d8 | 8.17 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenol, 2-propyl- | 136 | C9H12O | 000644-35-9 | 49 |
| 2 | Phenol, 2-ethyl-4-methyl- | 136 | C9H12O | 003855-26-3 | 47 |
| 3 | Phenol, 2,3,5-trimethyl- | 136 | C9H12O | 000697-82-5 | 47 |
| 4 | Phenol, 4-propyl- | 136 | C9H12O | 000645-56-7 | 46 |
| 5 | Phenol, 3,4,5-trimethyl- | 136 | C9H12O | 000527-54-8 | 46 |



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Acq On : 7 Jan 2019 17:26
Operator : JU/SJ
Sample : K1053-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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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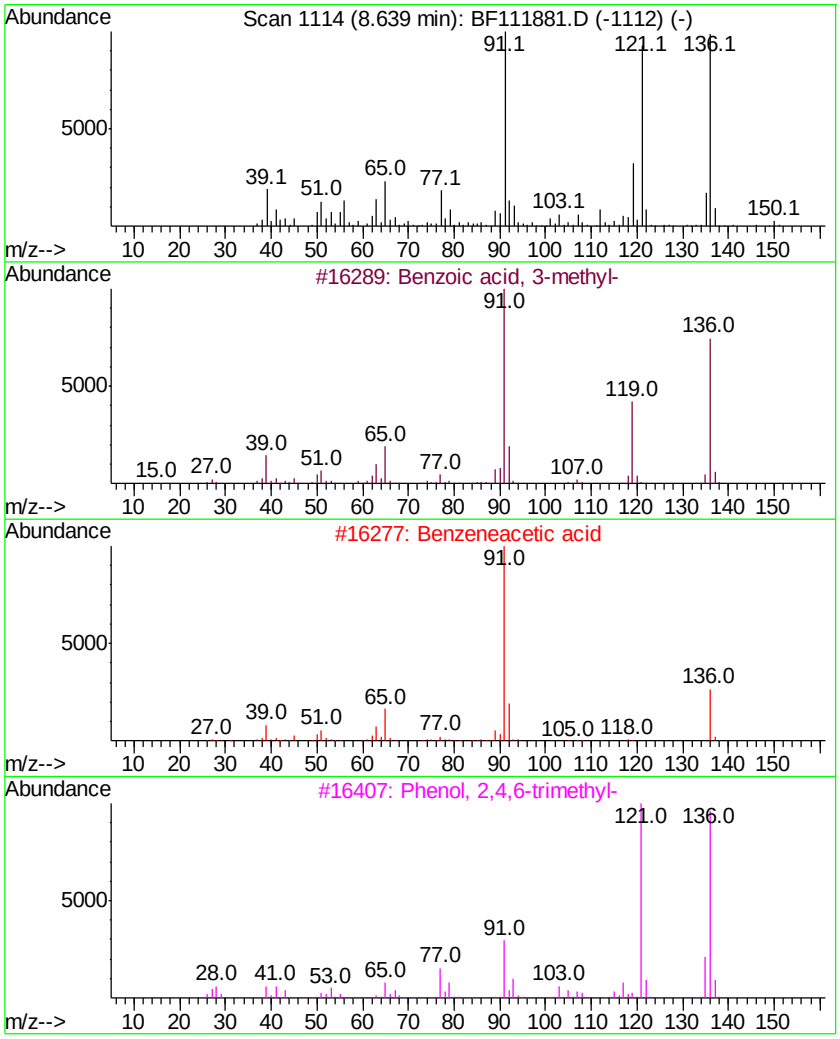
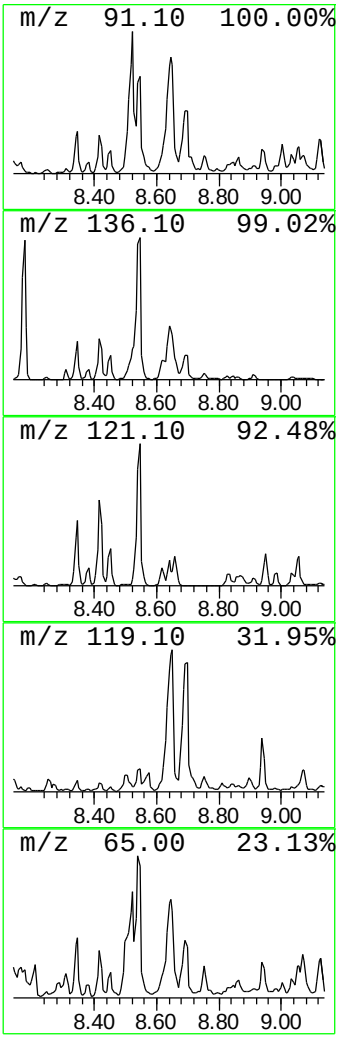
Peak Number 13 Benzoic acid, 3-methyl- Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.64 | 21.02 ng | 1504870 | Naphthalene-d8 | 8.17 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzoic acid, 3-methyl- | 136 | C8H8O2 | 000099-04-7 | 91 |
| 2 | Benzeneacetic acid | 136 | C8H8O2 | 000103-82-2 | 86 |
| 3 | Phenol, 2,4,6-trimethyl- | 136 | C9H12O | 000527-60-6 | 76 |
| 4 | Phenol, 2,3,6-trimethyl- | 136 | C9H12O | 002416-94-6 | 76 |
| 5 | 2,4-Dimethylanisole | 136 | C9H12O | 006738-23-4 | 74 |



Library Search Compound Report

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Data File : BF111881.D
Acq On : 7 Jan 2019 17:26
Operator : JU/SJ
Sample : K1053-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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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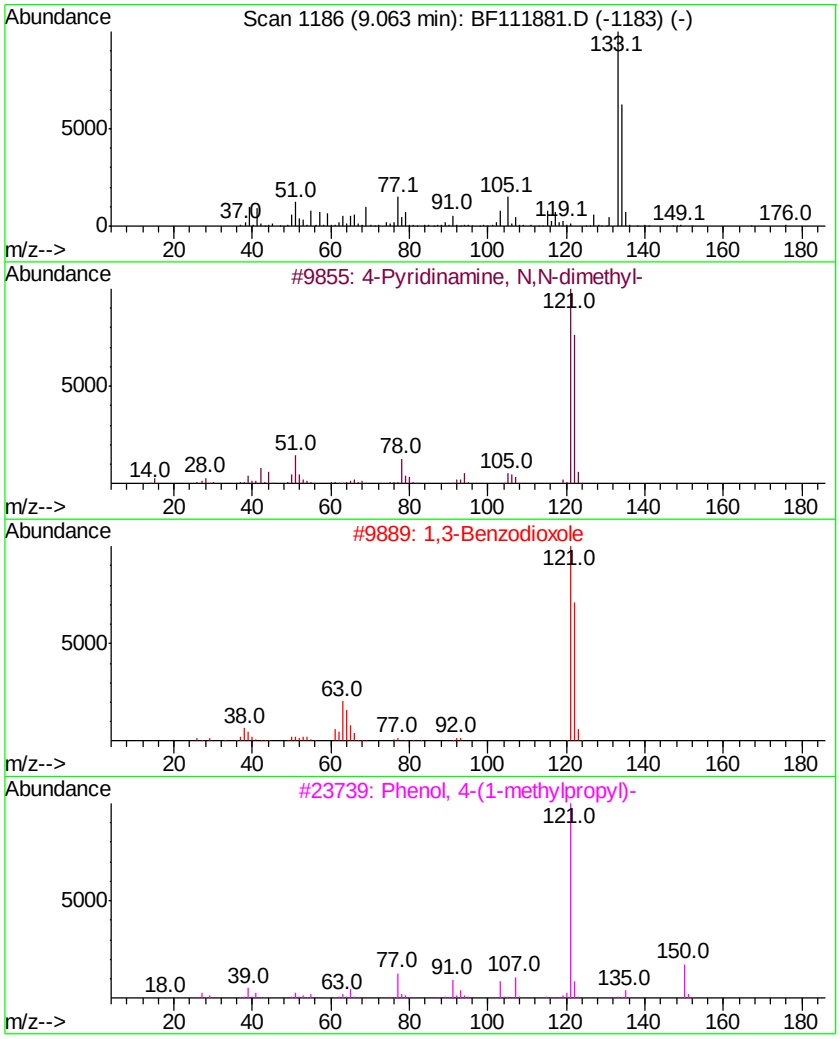
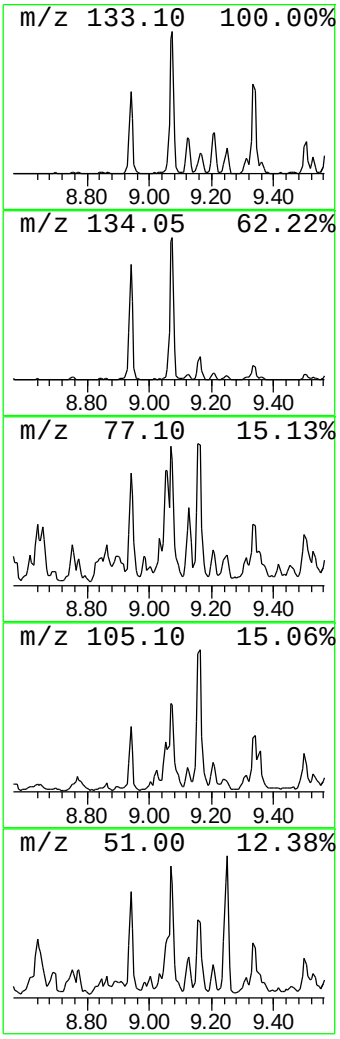
Peak Number 14 unknown9.06 Concentration Rank 18

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.06 | 15.55 ng | 875789 | Acenaphthene-d10 | 9.93 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-Pyridinamine, N,N-dimethyl- | 122 | C7H10N2 | 001122-58-3 | 46 |
| 2 | 1,3-Benzodioxole | 122 | C7H6O2 | 000274-09-9 | 43 |
| 3 | Phenol, 4-(1-methylpropyl)- | 150 | C10H14O | 000099-71-8 | 43 |
| 4 | Phenol, 2-(1-methylpropyl)- | 150 | C10H14O | 000089-72-5 | 38 |
| 5 | 2-Methyl-6-propylphenol | 150 | C10H14O | 003520-52-3 | 35 |



Library Search Compound Report

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Acq On : 7 Jan 2019 17:26
Operator : JU/SJ
Sample : K1053-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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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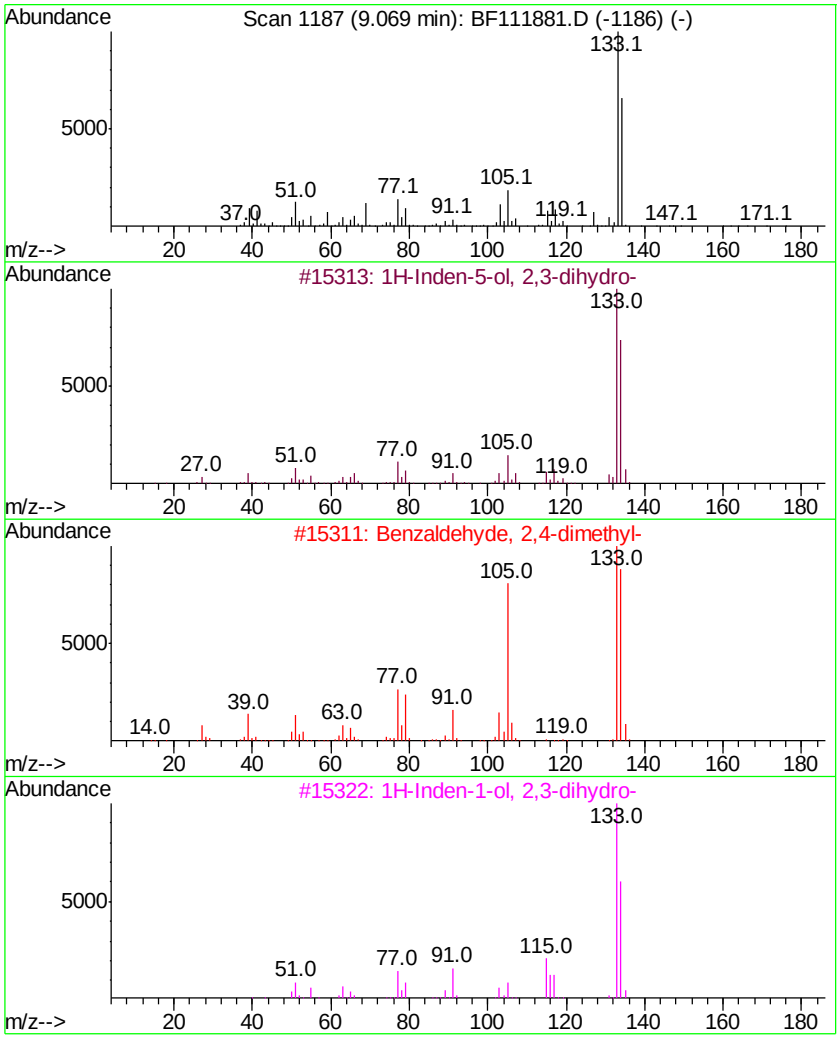
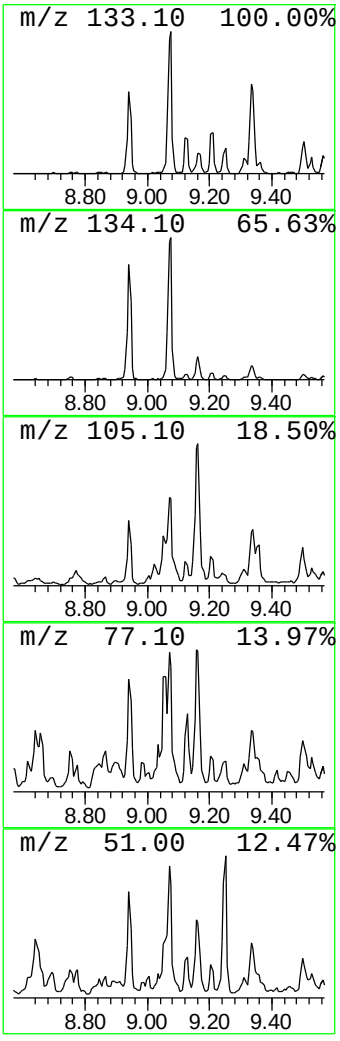
Peak Number 15 1H-Inden-5-ol, 2,3-dihydro- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.07 | 27.10 ng | 1526570 | Acenaphthene-d10 | 9.93 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1H-Inden-5-ol, 2,3-dihydro- | 134 | C9H10O | 001470-94-6 | 87 |
| 2 | Benzaldehyde, 2,4-dimethyl- | 134 | C9H10O | 015764-16-6 | 72 |
| 3 | 1H-Inden-1-ol, 2,3-dihydro- | 134 | C9H10O | 006351-10-6 | 64 |
| 4 | Oxalamide, N-(2-hydroxyethyl)-N'... | 278 | C14H18N2O4 | 1000304-26-2 | 50 |
| 5 | Propionitrile, 3-[(isochroman-1-... | 216 | C13H16N2O | 1000302-78-5 | 50 |



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Data File : BF111881.D
Acq On : 7 Jan 2019 17:26
Operator : JU/SJ
Sample : K1053-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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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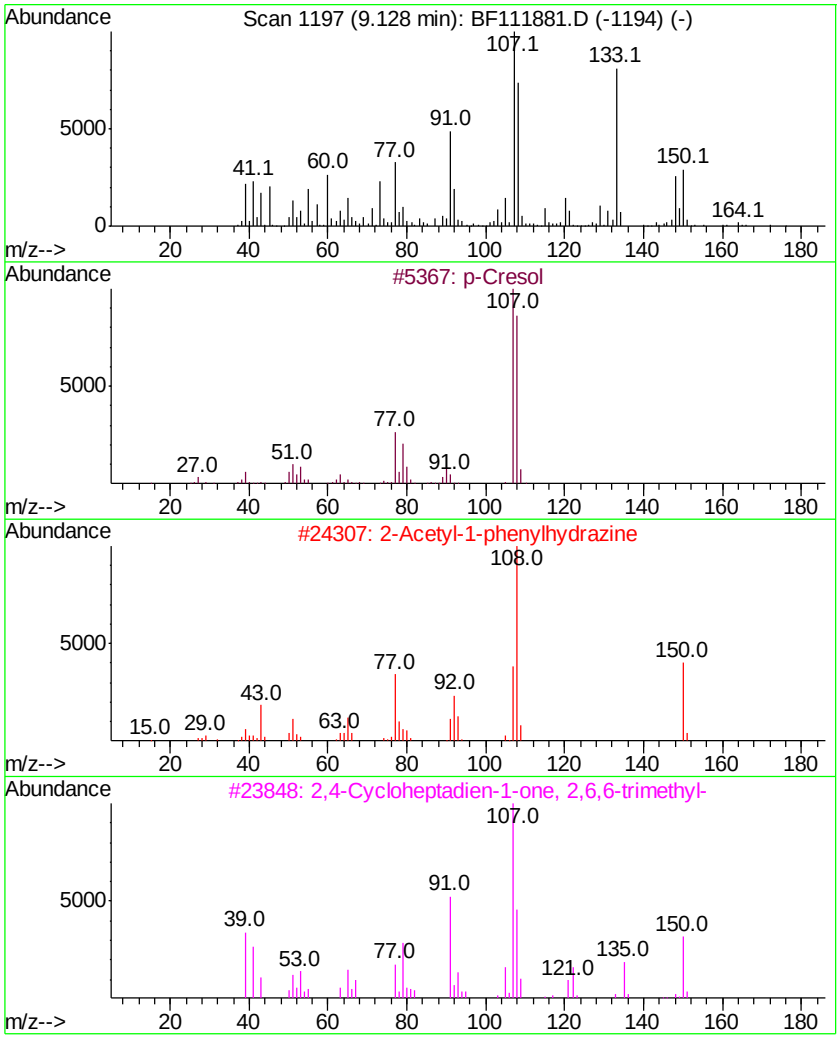
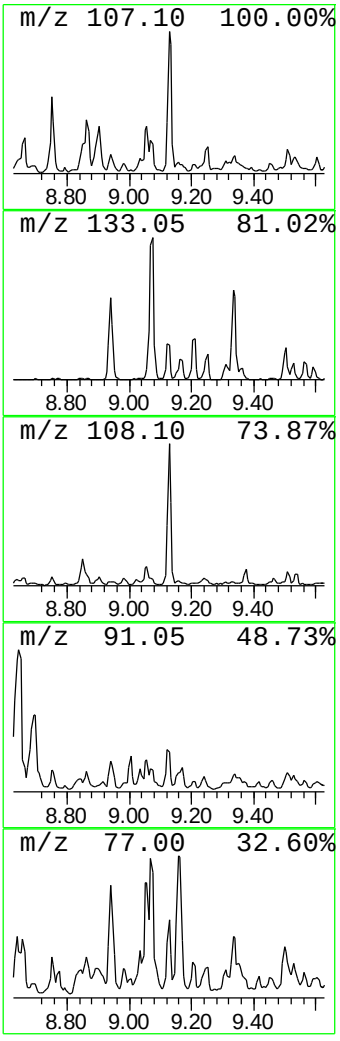
Peak Number 16 unknown9.13 Concentration Rank 17

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.13 | 16.15 ng | 909888 | Acenaphthene-d10 | 9.93 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | p-Cresol | 108 | C7H8O | 000106-44-5 | 41 |
| 2 | 2-Acetyl-1-phenylhydrazine | 150 | C8H10N2O | 000114-83-0 | 38 |
| 3 | 2,4-Cycloheptadien-1-one, 2,6,6-... | 150 | C10H14O | 000503-93-5 | 25 |
| 4 | 2-Aminoacetanilide | 150 | C8H10N2O | 034801-09-7 | 25 |
| 5 | Pyridine, 2,4-dimethyl- | 107 | C7H9N | 000108-47-4 | 20 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
Data File : BF111881.D
Acq On : 7 Jan 2019 17:26
Operator : JU/SJ
Sample : K1053-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

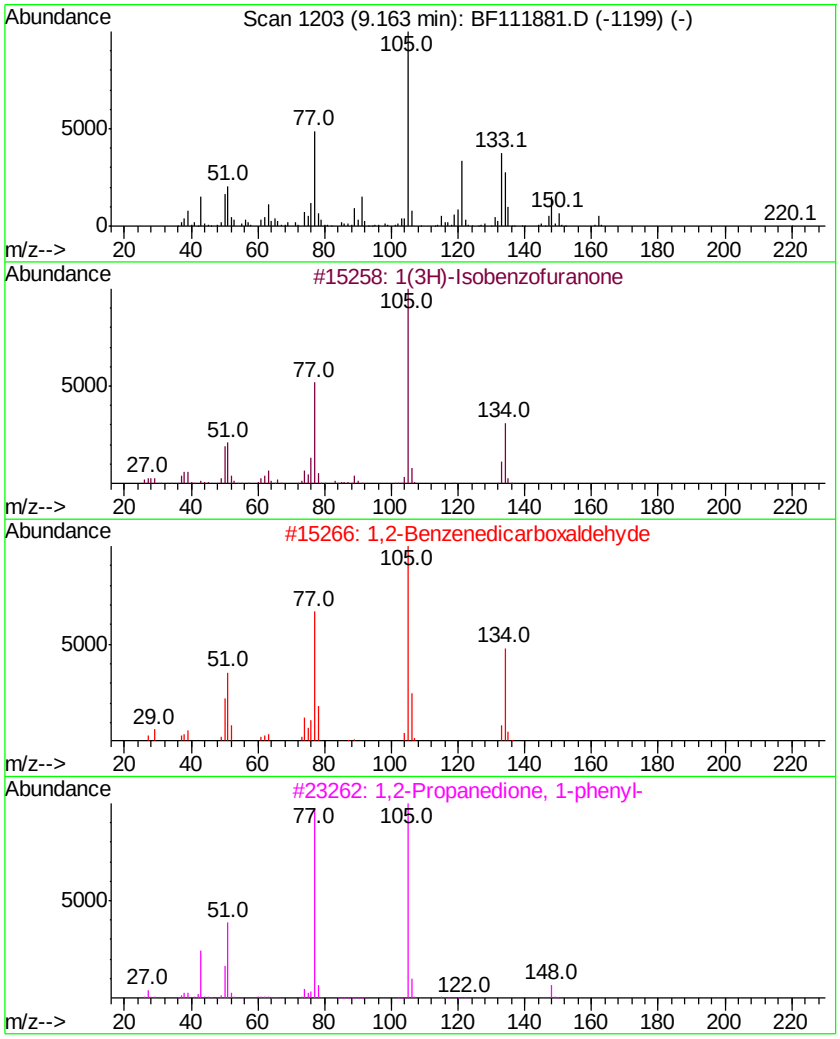
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

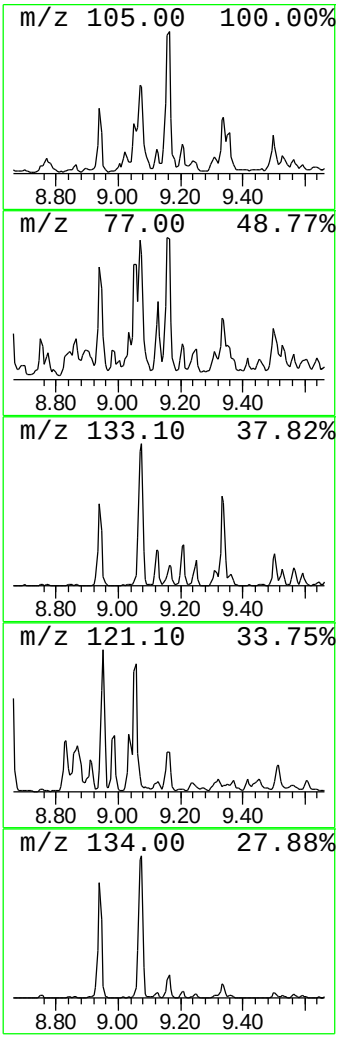
**********

Peak Number 17 1(3H)-Isobenzofuranone Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.16 | 20.41 ng | 1149580 | Acenaphthene-d10 | 9.93 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1(3H)-Isobenzofuranone | 134 | C8H6O2 | 000087-41-2 | 68 |
| 2 | 1,2-Benzenedicarboxaldehyde | 134 | C8H6O2 | 000643-79-8 | 58 |
| 3 | 1,2-Propanedione, 1-phenyl- | 148 | C9H8O2 | 000579-07-7 | 46 |
| 4 | 3H-Indazol-3-one, 1,2-dihydro- | 134 | C7H6N2O | 007364-25-2 | 46 |
| 5 | 1-Butanone, 1-phenyl- | 148 | C10H12O | 000495-40-9 | 43 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
Data File : BF111881.D
Acq On : 7 Jan 2019 17:26
Operator : JU/SJ
Sample : K1053-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

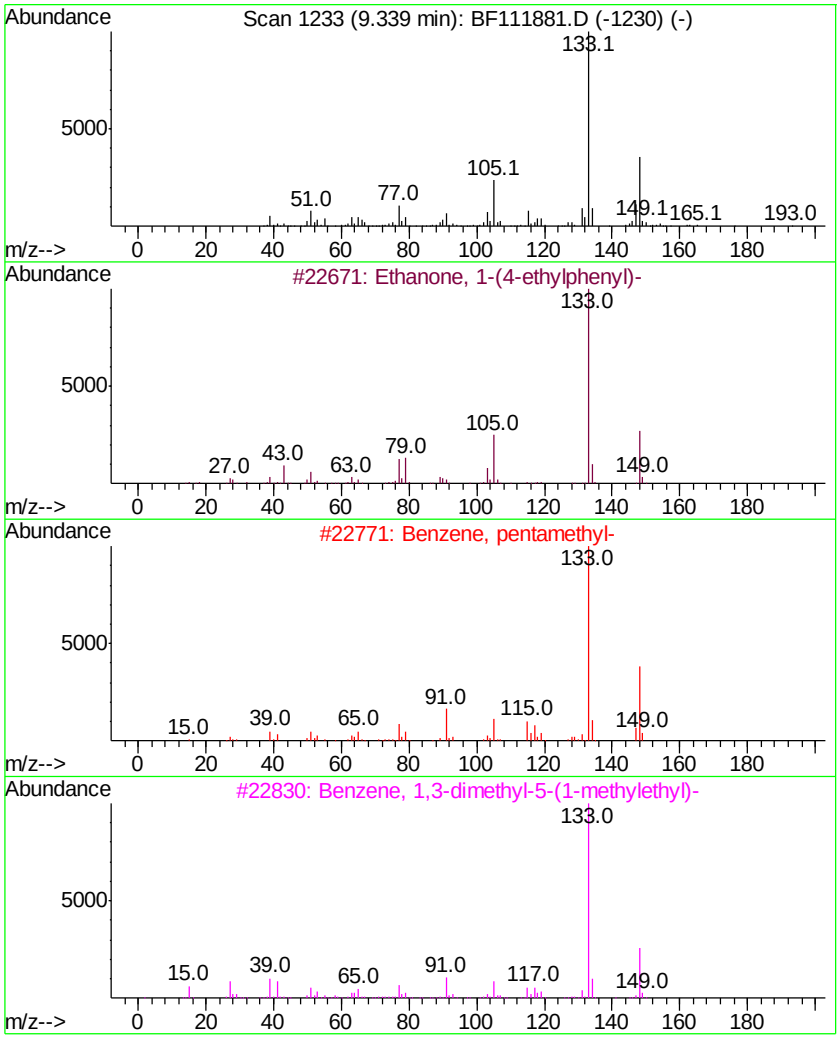
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

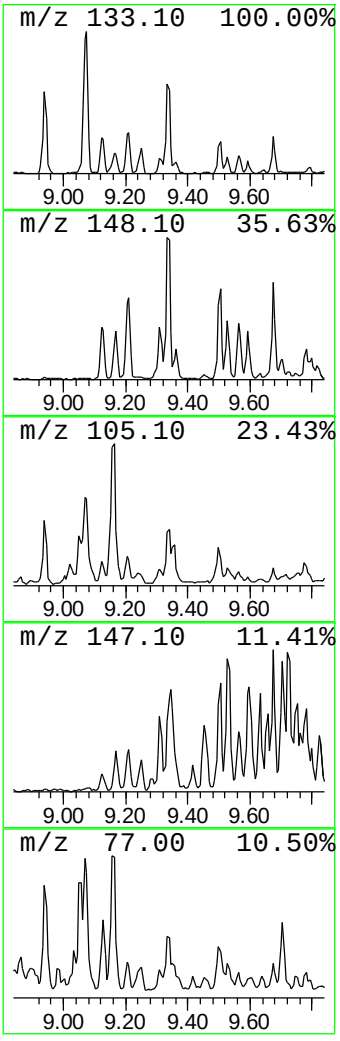
**********

Peak Number 18 Ethanone, 1-(4-ethylphenyl)- Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.34 | 18.01 ng | 1014430 | Acenaphthene-d10 | 9.93 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanone, 1-(4-ethylphenyl)- | 148 | C10H12O | 000937-30-4 | 81 |
| 2 | Benzene, pentamethyl- | 148 | C11H16 | 000700-12-9 | 72 |
| 3 | Benzene, 1,3-dimethyl-5-(1-methy... | 148 | C11H16 | 004706-90-5 | 59 |
| 4 | 1-Propanone, 2-chloro-1-(2,4-dim... | 210 | C12H15ClO | 054965-53-6 | 53 |
| 5 | 4-tert-Butyltoluene | 148 | C11H16 | 000098-51-1 | 53 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
Data File : BF111881.D
Acq On : 7 Jan 2019 17:26
Operator : JU/SJ
Sample : K1053-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

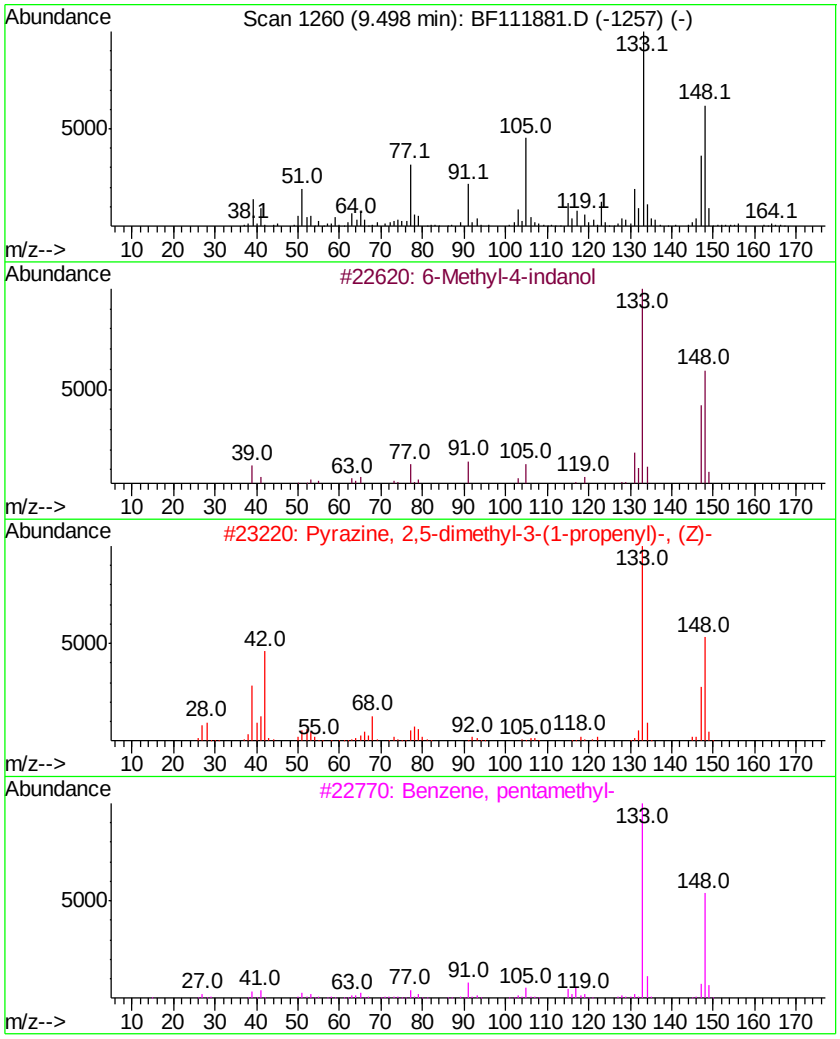
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

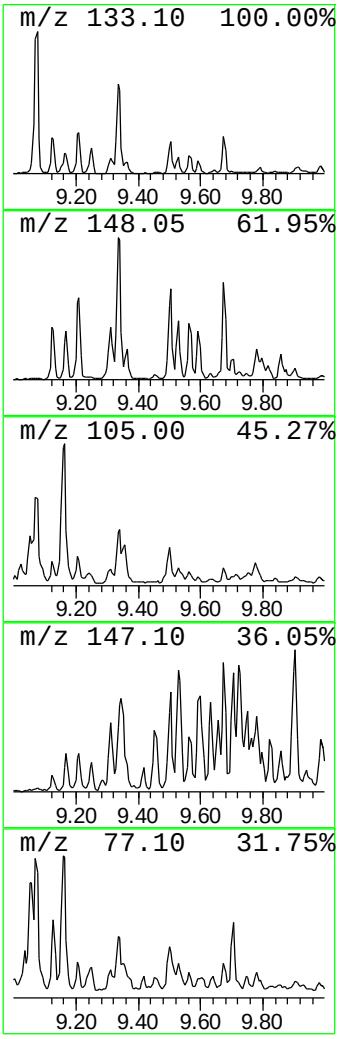
**********

Peak Number 19 6-Methyl-4-indanol Concentration Rank 20

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.50 | 14.71 ng | 828680 | Acenaphthene-d10 | 9.93 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 6-Methyl-4-indanol | 148 | C10H12O | 020294-32-0 | 94 |
| 2 | Pyrazine, 2,5-dimethyl-3-(1-prop... | 148 | C9H12N2 | 055138-73-3 | 72 |
| 3 | Benzene, pentamethyl- | 148 | C11H16 | 000700-12-9 | 62 |
| 4 | Benzene, 1-(1,1-dimethylethyl)-3... | 148 | C11H16 | 001075-38-3 | 58 |
| 5 | Benzene, 1,4-diethyl-2-methyl- | 148 | C11H16 | 013632-94-5 | 58 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010719\
Data File : BF111881.D
Acq On : 7 Jan 2019 17:26
Operator : JU/SJ
Sample : K1053-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

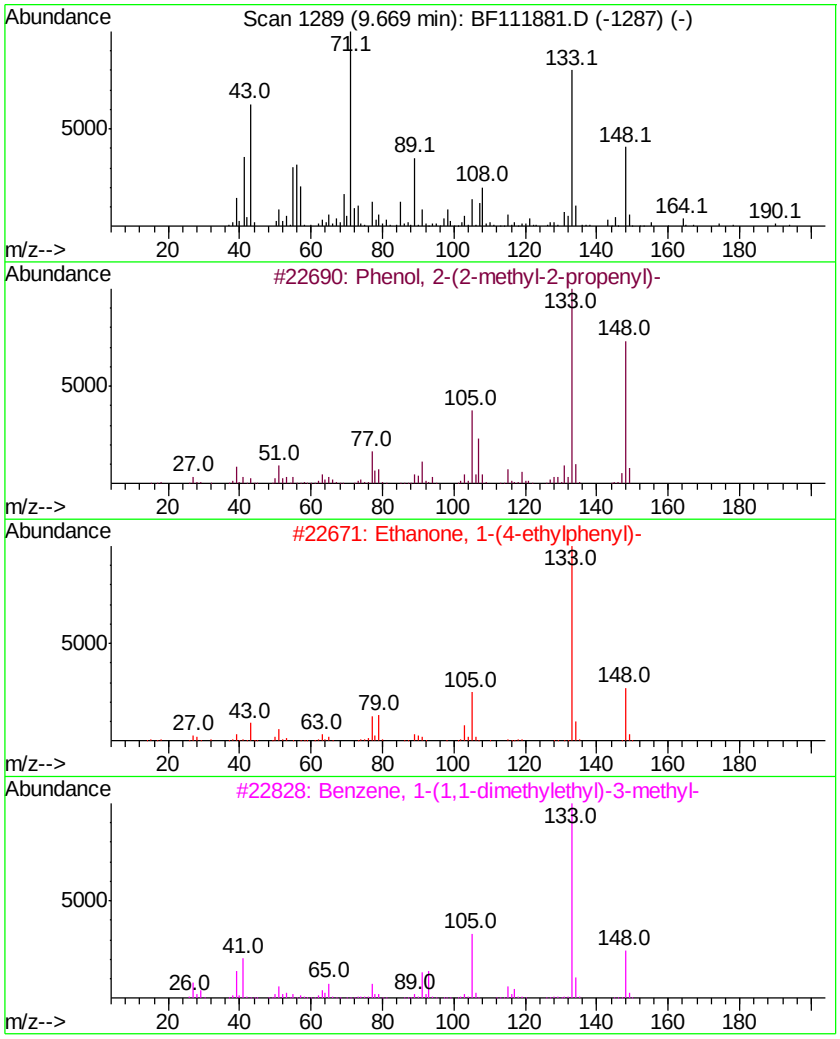
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

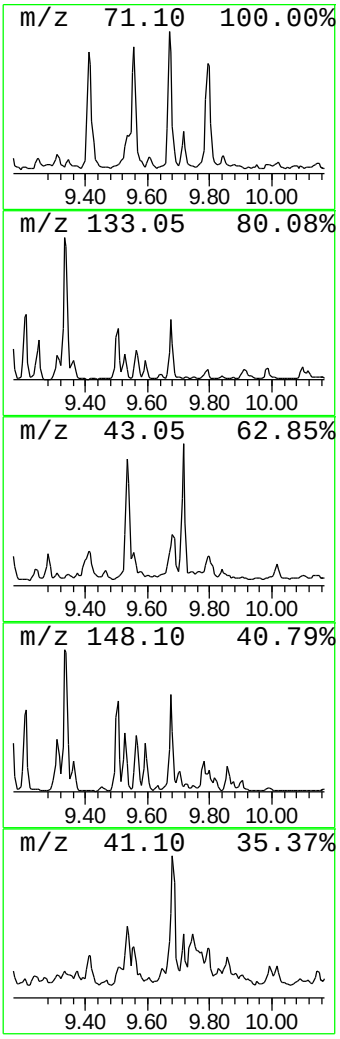
**********

Peak Number 20 Phenol, 2-(2-methyl-2-prope... Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.67 | 17.36 ng | 978028 | Acenaphthene-d10 | 9.93 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenol, 2-(2-methyl-2-propenyl)- | 148 | C10H12O | 020944-88-1 | 64 |
| 2 | Ethanone, 1-(4-ethylphenyl)- | 148 | C10H12O | 000937-30-4 | 49 |
| 3 | Benzene, 1-(1,1-dimethylethyl)-3... | 148 | C11H16 | 001075-38-3 | 49 |
| 4 | 5H-Cyclopentapyrazine, 6,7-dihyd... | 148 | C9H12N2 | 038917-61-2 | 49 |
| 5 | Benzene, 1,3-dimethyl-5-(1-methy... | 148 | C11H16 | 004706-90-5 | 46 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF010719\
Data File : BF111881.D
Acq On : 7 Jan 2019 17:26
Operator : JU/SJ
Sample : K1053-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMP-2-DRUM

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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 |
| Butanoic acid, 3-... | 5.72 | 35.6 | ng | 2462670 | 1 | 6.89 | 1384170 | 20.0 |
| Ethanol, 2-butoxy- | 5.90 | 20.5 | ng | 1416800 | 1 | 6.89 | 1384170 | 20.0 |
| Hexylene glycol | 6.18 | 16.3 | ng | 1125680 | 1 | 6.89 | 1384170 | 20.0 |
| 1-Hexanol, 2-ethyl- | 6.97 | 76.2 | ng | 5272860 | 1 | 6.89 | 1384170 | 20.0 |
| Hexanoic acid, 2-... | 7.73 | 44.2 | ng | 3163980 | 2 | 8.17 | 1431750 | 20.0 |
| unknown8.10 | 8.10 | 17.2 | ng | 1229660 | 2 | 8.17 | 1431750 | 20.0 |
| unknown8.28 | 8.28 | 26.4 | ng | 1891580 | 2 | 8.17 | 1431750 | 20.0 |
| unknown8.31 | 8.31 | 41.8 | ng | 2989290 | 2 | 8.17 | 1431750 | 20.0 |
| Phenol, 4-(1-meth... | 8.35 | 17.1 | ng | 1223130 | 2 | 8.17 | 1431750 | 20.0 |
| Phenol, 4-ethyl-3... | 8.42 | 15.1 | ng | 1081150 | 2 | 8.17 | 1431750 | 20.0 |
| unknown8.54 | 8.54 | 59.8 | ng | 4281400 | 2 | 8.17 | 1431750 | 20.0 |
| Benzoic acid, 3-m... | 8.64 | 21.0 | ng | 1504870 | 2 | 8.17 | 1431750 | 20.0 |
| unknown9.06 | 9.06 | 15.6 | ng | 875789 | 3 | 9.93 | 1126470 | 20.0 |
| 1H-Inden-5-ol, 2,... | 9.07 | 27.1 | ng | 1526570 | 3 | 9.93 | 1126470 | 20.0 |
| unknown9.13 | 9.13 | 16.1 | ng | 909888 | 3 | 9.93 | 1126470 | 20.0 |
| 1(3H)-Isobenzofur... | 9.16 | 20.4 | ng | 1149580 | 3 | 9.93 | 1126470 | 20.0 |
| Ethanone, 1-(4-et... | 9.34 | 18.0 | ng | 1014430 | 3 | 9.93 | 1126470 | 20.0 |
| 6-Methyl-4-indanol | 9.50 | 14.7 | ng | 828680 | 3 | 9.93 | 1126470 | 20.0 |
| Phenol, 2-(2-meth... | 9.67 | 17.4 | ng | 978028 | 3 | 9.93 | 1126470 | 20.0 |