LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106422.D
Acq On : 14 Jun 2018 5:43
Operator : JU/SJ
Sample : J3398-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** W-15

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-BF061118.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 | 3.978 | 274 | 279 | 287 | rBV | 60969 | 84934 | 1.49% | 0.127% |
| 2 | 5.190 | 481 | 485 | 492 | rVB | 106693 | 113961 | 2.00% | 0.171% |
| 3 | 5.613 | 553 | 557 | 564 | rBV | 1489602 | 1626433 | 28.61% | 2.435% |
| 4 | 6.613 | 724 | 727 | 735 | rVB | 949915 | 1064936 | 18.73% | 1.594% |
| 5 | 6.748 | 746 | 750 | 753 | rBV | 3057602 | 2787992 | 49.04% | 4.174% |
| 6 | 6.966 | 783 | 787 | 790 | rVV | 1069286 | 899956 | 15.83% | 1.347% |
| 7 | 7.019 | 794 | 796 | 800 | rVB | 86911 | 74123 | 1.30% | 0.111% |
| 8 | 7.125 | 809 | 814 | 816 | rBV | 2937016 | 2832065 | 49.81% | 4.240% |
| 9 | 7.143 | 816 | 817 | 821 | rVV | 467143 | 331719 | 5.83% | 0.497% |
| 10 | 7.207 | 825 | 828 | 830 | rVV | 138728 | 98278 | 1.73% | 0.147% |
| 11 | 7.301 | 841 | 844 | 848 | rVB | 162949 | 152809 | 2.69% | 0.229% |
| 12 | 7.360 | 851 | 854 | 862 | rVB4 | 81424 | 97245 | 1.71% | 0.146% |
| 13 | 7.495 | 873 | 877 | 879 | rBV | 376105 | 320484 | 5.64% | 0.480% |
| 14 | 7.531 | 879 | 883 | 886 | rVB | 2636520 | 2630886 | 46.27% | 3.939% |
| 15 | 7.607 | 892 | 896 | 900 | rBV6 | 137426 | 185748 | 3.27% | 0.278% |
| 16 | 7.648 | 900 | 903 | 907 | rVB | 129733 | 114540 | 2.01% | 0.171% |
| 17 | 7.701 | 907 | 912 | 914 | rBV4 | 64762 | 103644 | 1.82% | 0.155% |
| 18 | 7.731 | 914 | 917 | 919 | rVV | 246037 | 213914 | 3.76% | 0.320% |
| 19 | 7.766 | 920 | 923 | 927 | rVB2 | 105593 | 130772 | 2.30% | 0.196% |
| 20 | 7.807 | 927 | 930 | 934 | rBV3 | 94680 | 100971 | 1.78% | 0.151% |
| 21 | 7.901 | 942 | 946 | 953 | rVB4 | 479457 | 742267 | 13.06% | 1.111% |
| 22 | 7.984 | 955 | 960 | 968 | rBV | 1409807 | 1431459 | 25.18% | 2.143% |
| 23 | 8.048 | 968 | 971 | 975 | rVV4 | 102097 | 167930 | 2.95% | 0.251% |
| 24 | 8.084 | 975 | 977 | 979 | rVB2 | 90853 | 73997 | 1.30% | 0.111% |
| 25 | 8.154 | 983 | 989 | 991 | rBV5 | 102066 | 165607 | 2.91% | 0.248% |
| 26 | 8.178 | 991 | 993 | 996 | rVV2 | 275075 | 232562 | 4.09% | 0.348% |
| 27 | 8.248 | 999 | 1005 | 1007 | rVV | 1394520 | 1333212 | 23.45% | 1.996% |
| 28 | 8.290 | 1010 | 1012 | 1015 | rVB2 | 153958 | 117417 | 2.07% | 0.176% |
| 29 | 8.331 | 1015 | 1019 | 1022 | rVB3 | 101667 | 105377 | 1.85% | 0.158% |
| 30 | 8.442 | 1036 | 1038 | 1043 | rVB2 | 123783 | 165265 | 2.91% | 0.247% |
| 31 | 8.490 | 1043 | 1046 | 1050 | rBV3 | 224103 | 275524 | 4.85% | 0.413% |
| 32 | 8.625 | 1066 | 1069 | 1072 | rVB3 | 129295 | 132925 | 2.34% | 0.199% |
| 33 | 8.654 | 1072 | 1074 | 1077 | rBV2 | 148528 | 113205 | 1.99% | 0.169% |
| 34 | 8.713 | 1081 | 1084 | 1088 | rBV3 | 152764 | 177755 | 3.13% | 0.266% |

LSC Area Percent Report

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Data File : BF106422.D
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Operator : JU/SJ
Sample : J3398-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** W-15

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-BF061118.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 8.748 | 1088 | 1090 | 1095 | rVB4 | 125386 | 102245 | 1.80% | 0.153% |
| 36 | 8.837 | 1103 | 1105 | 1109 | rVB4 | 111425 | 121392 | 2.14% | 0.182% |
| 37 | 8.878 | 1109 | 1112 | 1115 | rBV3 | 101978 | 151556 | 2.67% | 0.227% |
| 38 | 8.907 | 1115 | 1117 | 1119 | rVB | 265730 | 175714 | 3.09% | 0.263% |
| 39 | 8.937 | 1119 | 1122 | 1124 | rVB3 | 86976 | 80910 | 1.42% | 0.121% |
| 40 | 8.960 | 1124 | 1126 | 1129 | rBV | 157990 | 165360 | 2.91% | 0.248% |
| 41 | 9.007 | 1129 | 1134 | 1136 | rBV2 | 302519 | 396167 | 6.97% | 0.593% |
| 42 | 9.031 | 1136 | 1138 | 1140 | rVV2 | 115075 | 107018 | 1.88% | 0.160% |
| 43 | 9.060 | 1140 | 1143 | 1149 | rVB3 | 483849 | 546651 | 9.61% | 0.818% |
| 44 | 9.107 | 1149 | 1151 | 1155 | rVB4 | 99467 | 99271 | 1.75% | 0.149% |
| 45 | 9.154 | 1155 | 1159 | 1163 | rBV6 | 349980 | 425607 | 7.49% | 0.637% |
| 46 | 9.189 | 1163 | 1165 | 1169 | rBV3 | 193701 | 189907 | 3.34% | 0.284% |
| 47 | 9.248 | 1172 | 1175 | 1178 | rVB | 498725 | 405283 | 7.13% | 0.607% |
| 48 | 9.289 | 1178 | 1182 | 1184 | rBV3 | 178992 | 224983 | 3.96% | 0.337% |
| 49 | 9.325 | 1184 | 1188 | 1191 | rVB | 4015003 | 3831742 | 67.39% | 5.737% |
| 50 | 9.366 | 1191 | 1195 | 1198 | rBV3 | 217729 | 314625 | 5.53% | 0.471% |
| 51 | 9.442 | 1201 | 1208 | 1210 | rBV5 | 240593 | 436986 | 7.69% | 0.654% |
| 52 | 9.466 | 1210 | 1212 | 1214 | rVB2 | 108922 | 81068 | 1.43% | 0.121% |
| 53 | 9.489 | 1214 | 1216 | 1219 | rVB | 194302 | 140131 | 2.46% | 0.210% |
| 54 | 9.519 | 1219 | 1221 | 1224 | rVB2 | 105659 | 97462 | 1.71% | 0.146% |
| 55 | 9.572 | 1225 | 1230 | 1235 | rBV4 | 349158 | 651031 | 11.45% | 0.975% |
| 56 | 9.613 | 1235 | 1237 | 1239 | rBV3 | 83486 | 75893 | 1.33% | 0.114% |
| 57 | 9.648 | 1239 | 1243 | 1244 | rBV3 | 177359 | 248149 | 4.36% | 0.372% |
| 58 | 9.684 | 1244 | 1249 | 1251 | rVV2 | 551768 | 856508 | 15.06% | 1.282% |
| 59 | 9.707 | 1251 | 1253 | 1257 | rVV2 | 282221 | 292668 | 5.15% | 0.438% |
| 60 | 9.748 | 1257 | 1260 | 1265 | rVB5 | 471372 | 664485 | 11.69% | 0.995% |
| 61 | 9.795 | 1265 | 1268 | 1270 | rVB2 | 84162 | 84548 | 1.49% | 0.127% |
| 62 | 9.889 | 1278 | 1284 | 1286 | rBV3 | 331700 | 392638 | 6.91% | 0.588% |
| 63 | 9.919 | 1286 | 1289 | 1291 | rBV2 | 252195 | 253366 | 4.46% | 0.379% |
| 64 | 9.948 | 1291 | 1294 | 1298 | rVB3 | 231084 | 322733 | 5.68% | 0.483% |
| 65 | 10.007 | 1300 | 1304 | 1312 | rBV2 | 1623825 | 1822033 | 32.05% | 2.728% |
| 66 | 10.089 | 1313 | 1318 | 1320 | rBV2 | 433803 | 607253 | 10.68% | 0.909% |
| 67 | 10.166 | 1325 | 1331 | 1335 | rBV5 | 491338 | 933646 | 16.42% | 1.398% |
| 68 | 10.278 | 1347 | 1350 | 1353 | rBV5 | 94635 | 149686 | 2.63% | 0.224% |
| 69 | 10.366 | 1354 | 1365 | 1367 | rVV2 | 2598946 | 5685537 | 100.00% | 8.512% |
| 70 | 10.407 | 1367 | 1372 | 1377 | rVB5 | 912045 | 1561460 | 27.46% | 2.338% |
| 71 | 10.489 | 1383 | 1386 | 1388 | rBV3 | 138133 | 174943 | 3.08% | 0.262% |

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Sample : J3398-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** W-15

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-BF061118.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 72 | 10.536 | 1388 | 1394 | 1399 | rVV3 | 1577478 | 3362983 | 59.15% | 5.035% |
| 73 | 10.607 | 1402 | 1406 | 1409 | rVV4 | 1012222 | 1370665 | 24.11% | 2.052% |
| 74 | 10.631 | 1409 | 1410 | 1413 | rVV | 277818 | 211908 | 3.73% | 0.317% |
| 75 | 10.660 | 1413 | 1415 | 1420 | rVB | 346367 | 404286 | 7.11% | 0.605% |
| 76 | 10.742 | 1423 | 1429 | 1431 | rBV2 | 554433 | 902786 | 15.88% | 1.352% |
| 77 | 10.772 | 1431 | 1434 | 1436 | rVV3 | 472030 | 557685 | 9.81% | 0.835% |
| 78 | 10.807 | 1436 | 1440 | 1442 | rVV | 2505061 | 2539389 | 44.66% | 3.802% |
| 79 | 10.848 | 1442 | 1447 | 1449 | rVV3 | 1128512 | 1598792 | 28.12% | 2.394% |
| 80 | 10.872 | 1449 | 1451 | 1455 | rVV3 | 577998 | 646346 | 11.37% | 0.968% |
| 81 | 10.925 | 1455 | 1460 | 1465 | rVB3 | 831142 | 1202729 | 21.15% | 1.801% |
| 82 | 10.978 | 1466 | 1469 | 1471 | rBV2 | 226386 | 279639 | 4.92% | 0.419% |
| 83 | 11.001 | 1471 | 1473 | 1477 | rVV3 | 390021 | 435692 | 7.66% | 0.652% |
| 84 | 11.042 | 1478 | 1480 | 1482 | rVB | 332453 | 263850 | 4.64% | 0.395% |
| 85 | 11.066 | 1482 | 1484 | 1486 | rBV | 170821 | 157259 | 2.77% | 0.235% |
| 86 | 11.136 | 1493 | 1496 | 1499 | rBV3 | 440403 | 592045 | 10.41% | 0.886% |
| 87 | 11.201 | 1502 | 1507 | 1511 | rBV4 | 422938 | 816215 | 14.36% | 1.222% |
| 88 | 11.236 | 1511 | 1513 | 1519 | rVB4 | 486700 | 614644 | 10.81% | 0.920% |
| 89 | 11.289 | 1520 | 1522 | 1524 | rBV | 126567 | 93973 | 1.65% | 0.141% |
| 90 | 11.325 | 1526 | 1528 | 1533 | rVB4 | 260201 | 322826 | 5.68% | 0.483% |
| 91 | 11.448 | 1546 | 1549 | 1554 | rVB5 | 151043 | 177956 | 3.13% | 0.266% |
| 92 | 11.501 | 1554 | 1558 | 1561 | rBV | 1318805 | 1209296 | 21.27% | 1.810% |
| 93 | 11.878 | 1620 | 1622 | 1627 | rVB2 | 190645 | 200545 | 3.53% | 0.300% |
| 94 | 12.019 | 1643 | 1646 | 1650 | rBV | 278430 | 252013 | 4.43% | 0.377% |
| 95 | 12.254 | 1681 | 1686 | 1690 | rBV | 1224858 | 1539180 | 27.07% | 2.304% |
| 96 | 12.801 | 1776 | 1779 | 1784 | rVB2 | 132632 | 144640 | 2.54% | 0.217% |
| 97 | 13.083 | 1823 | 1827 | 1830 | rBV | 3044874 | 2835092 | 49.86% | 4.245% |
| 98 | 14.142 | 2003 | 2007 | 2011 | rBV | 1045790 | 924611 | 16.26% | 1.384% |
| 99 | 14.995 | 2149 | 2152 | 2156 | rVB | 149247 | 148038 | 2.60% | 0.222% |
| 100 | 15.671 | 2262 | 2267 | 2277 | rVB | 707918 | 917981 | 16.15% | 1.374% |

Sum of corrected areas: 66793631

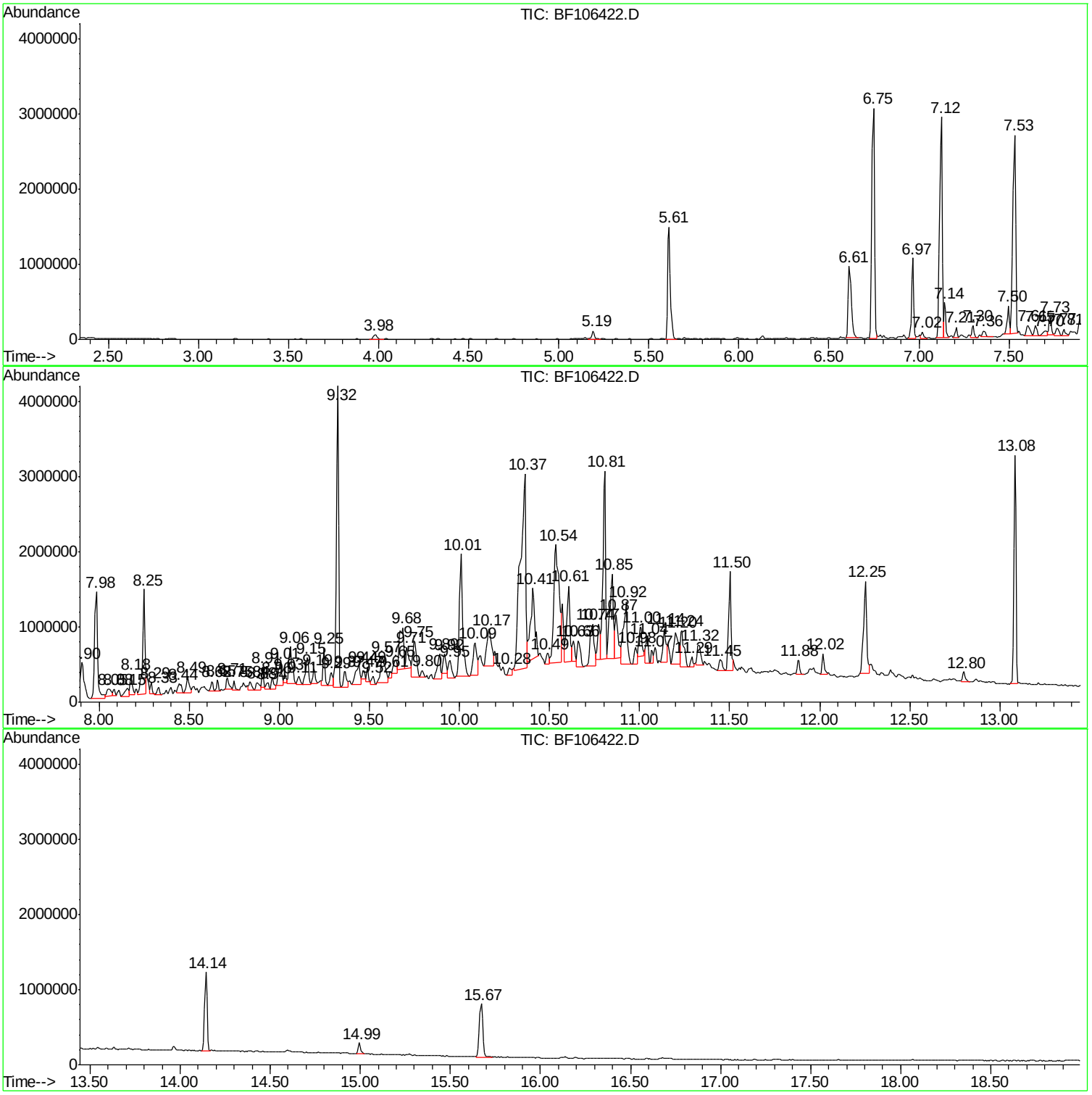
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106422.D
Acq On : 14 Jun 2018 5:43
Operator : JU/SJ
Sample : J3398-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** W-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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\BF061318\
Data File : BF106422.D
Acq On : 14 Jun 2018 5:43
Operator : JU/SJ
Sample : J3398-05
Misc :
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**Instrument :** BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

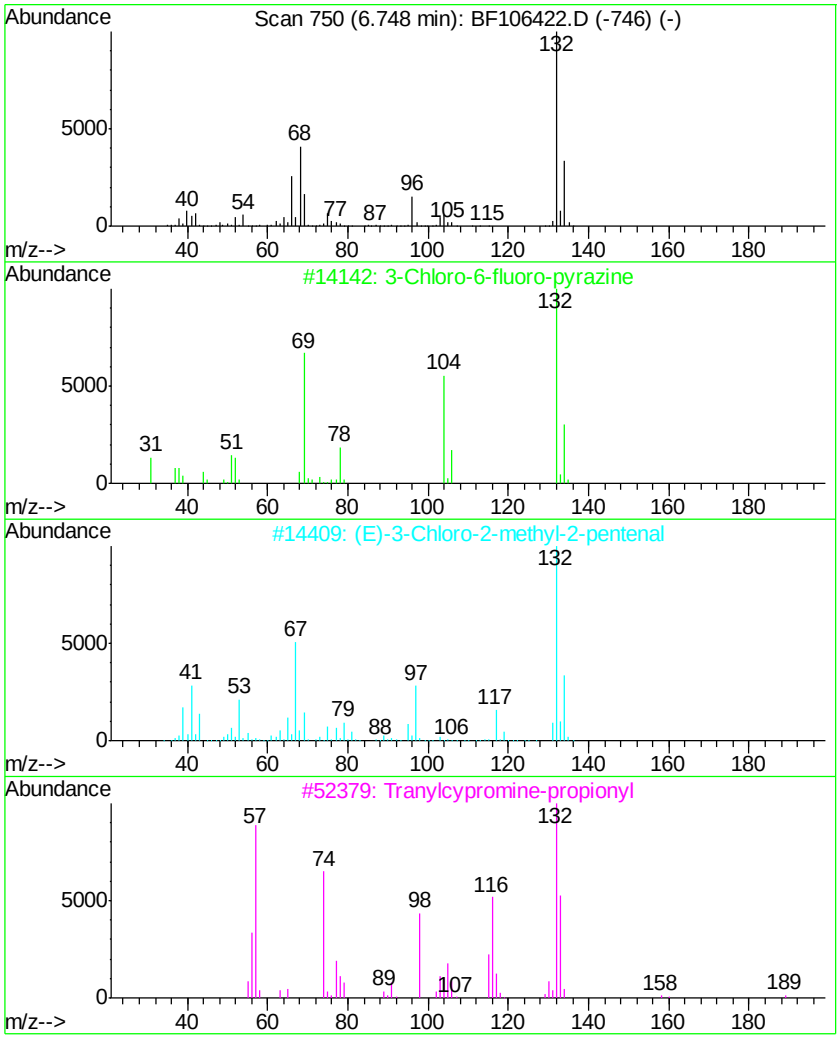
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

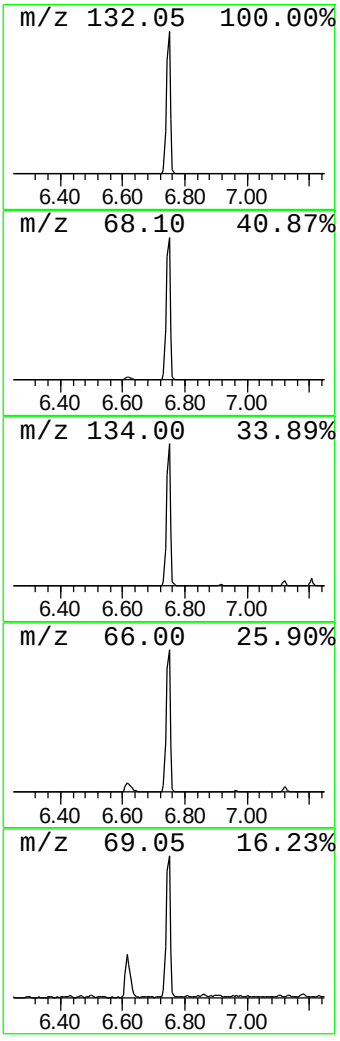
**********

Peak Number 1 unknown6.75 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.75 | 61.96 ng | 2787990 | 1,4-Dichlorobenzene-d4 | 6.97 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 16 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | 1,3,5-Trifluorobenzene | 132 | C6H3F3 | 000372-38-3 | 9 |
| 5 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |



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Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106422.D
Acq On : 14 Jun 2018 5:43
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

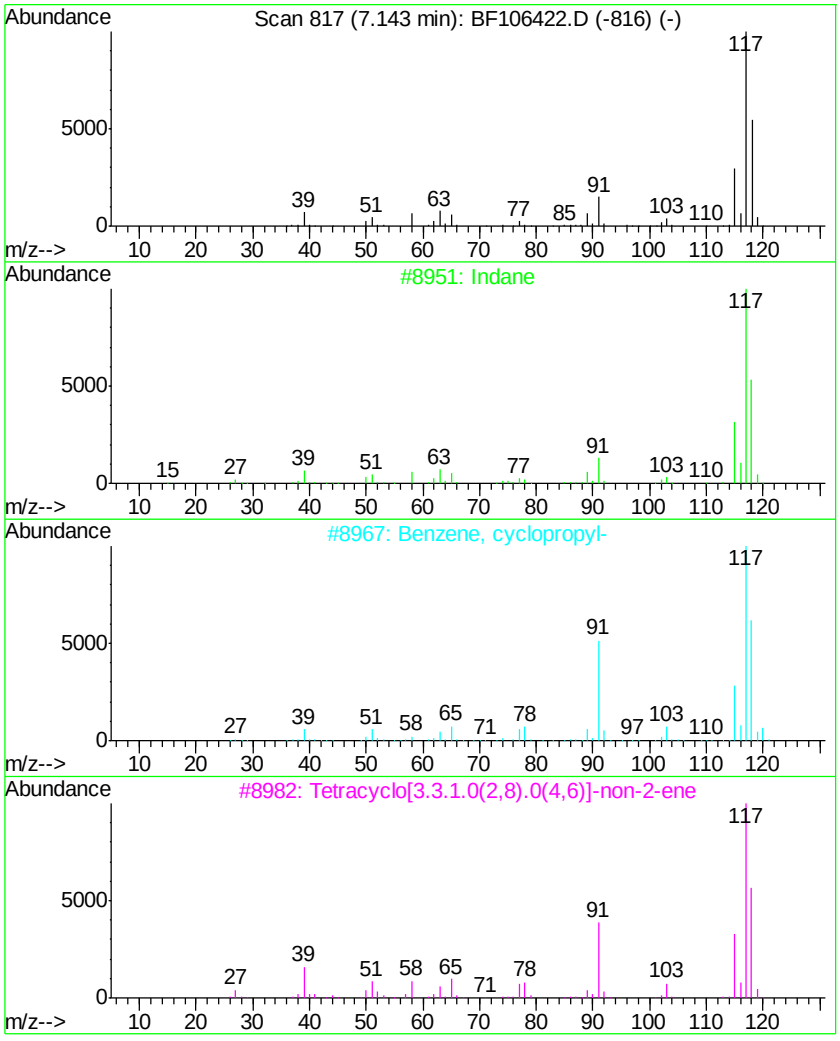
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

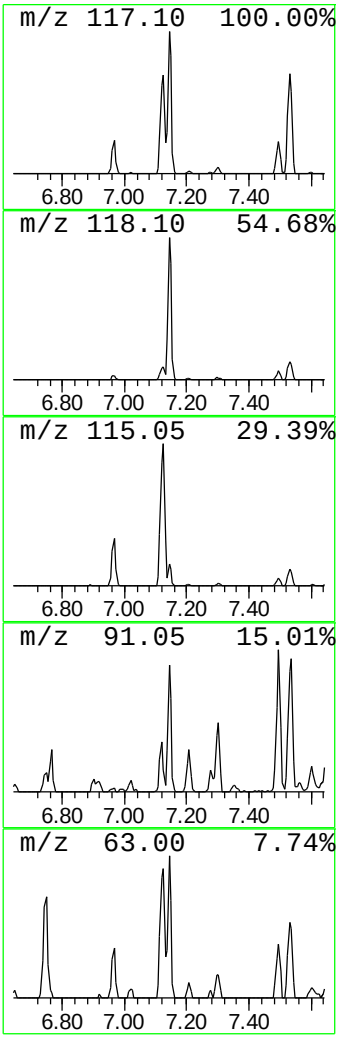
**********

Peak Number 3 Indane Concentration Rank 17

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.14 | 7.37 ng | 331719 | 1,4-Dichlorobenzene-d4 | 6.97 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Indane | 118 | C9H10 | 000496-11-7 | 87 |
| 2 | Benzene, cyclopropyl- | 118 | C9H10 | 000873-49-4 | 83 |
| 3 | Tetracyclo[3.3.1.0(2,8).0(4,6)]-... | 118 | C9H10 | 1000191-13-7 | 83 |
| 4 | trans-Cinnamyl bromide | 196 | C9H9Br | 026146-77-0 | 53 |
| 5 | Benzene, 2-propenyl- | 118 | C9H10 | 000300-57-2 | 53 |



# Library Search Compound Report

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

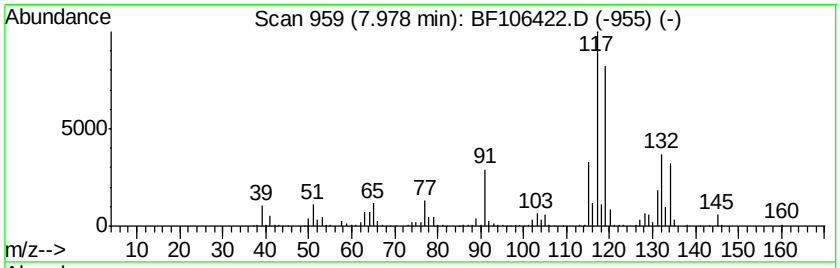
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

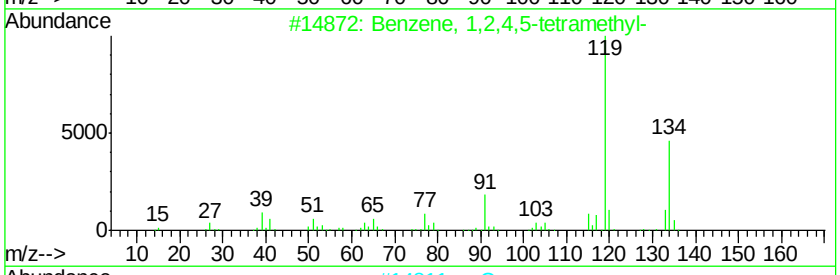
**********

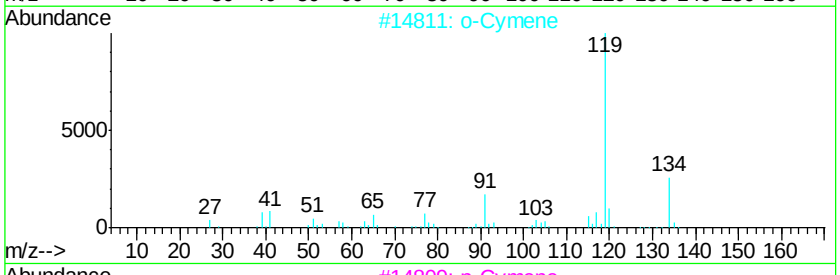
Peak Number 4 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 6

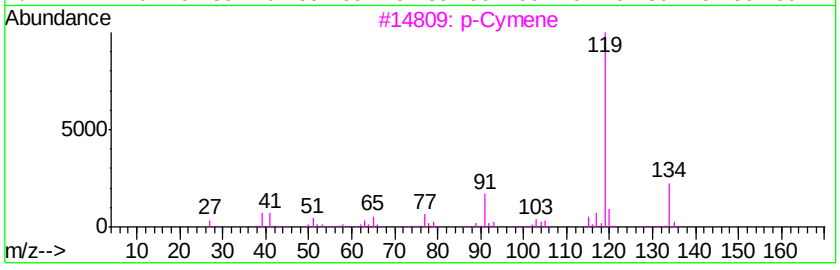
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.98 | 21.47 ng | 1431460 | Naphthalene-d8 | 8.25 |

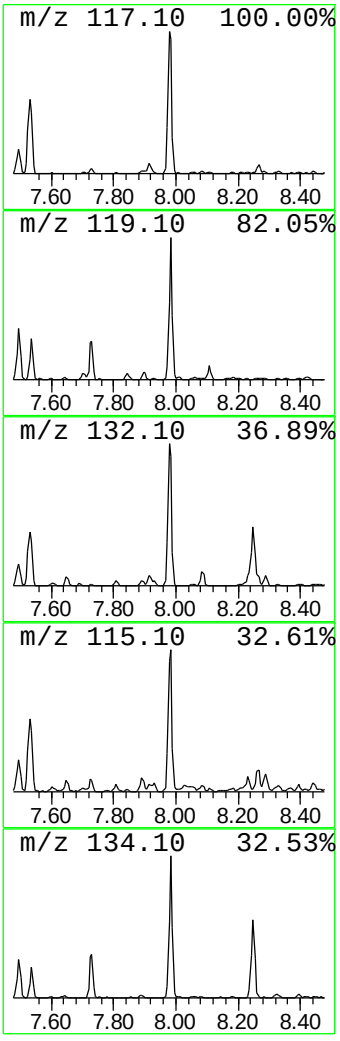
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzene, 1,2,4,5-tetramethyl- | 134 | C10H14 | 000095-93-2 | 64 |
| 2 | o-Cymene | 134 | C10H14 | 000527-84-4 | 60 |
| 3 | p-Cymene | 134 | C10H14 | 000099-87-6 | 60 |
| 4 | Benzene, 1-methyl-3-(1-methyleth... | 134 | C10H14 | 000535-77-3 | 60 |
| 5 | Benzene, 1-ethyl-2,4-dimethyl- | 134 | C10H14 | 000874-41-9 | 60 |



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Acq On : 14 Jun 2018 5:43
Operator : JU/SJ
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Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** W-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

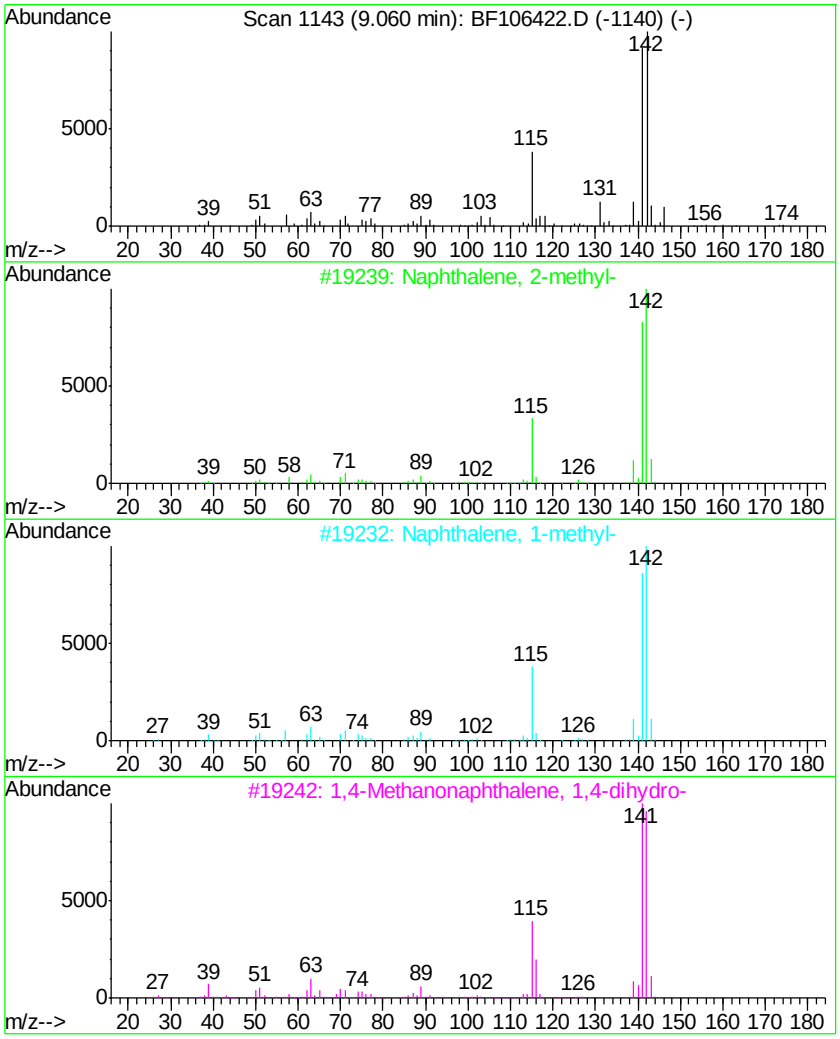
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

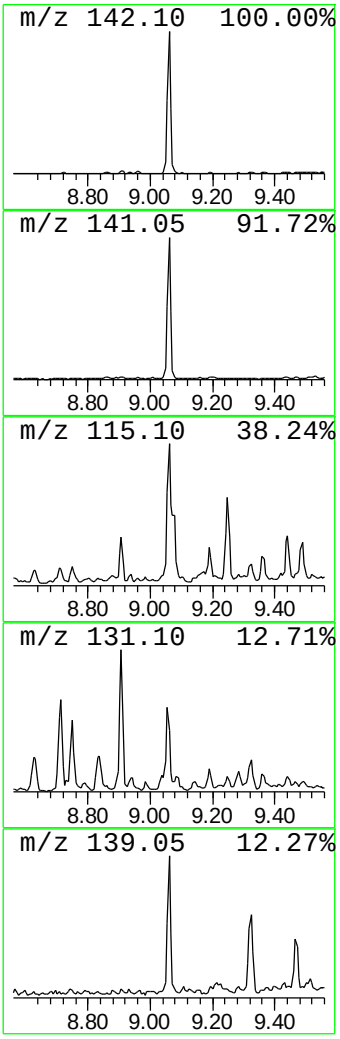
**********

Peak Number 5 Naphthalene, 1-methyl- Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.06 | 8.20 ng | 546651 | Naphthalene-d8 | 8.25 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Naphthalene, 2-methyl- | 142 | C11H10 | 000091-57-6 | 94 |
| 2 | Naphthalene, 1-methyl- | 142 | C11H10 | 000090-12-0 | 92 |
| 3 | 1,4-Methanonaphthalene, 1,4-dihy... | 142 | C11H10 | 004453-90-1 | 91 |
| 4 | Benzocycloheptatriene | 142 | C11H10 | 000264-09-5 | 87 |
| 5 | Bicyclo[4.4.1]undeca-1,3,5,7,9-p... | 142 | C11H10 | 002443-46-1 | 87 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106422.D
Acq On : 14 Jun 2018 5:43
Operator : JU/SJ
Sample : J3398-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** W-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

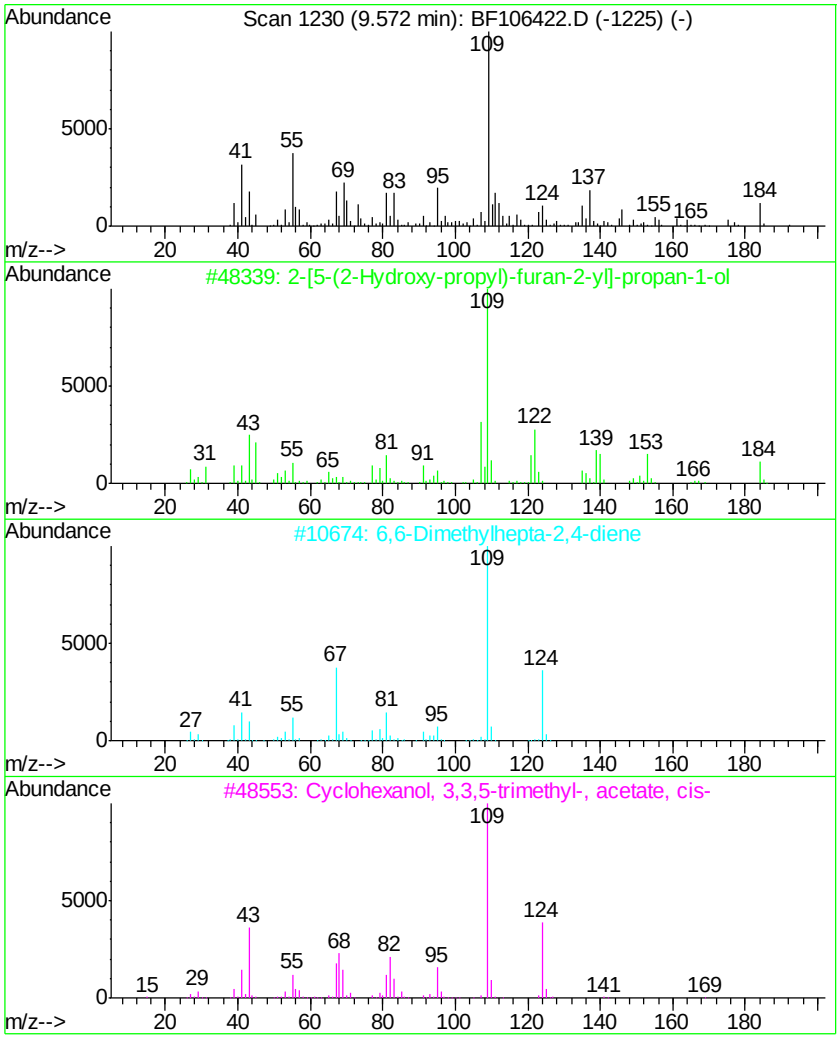
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

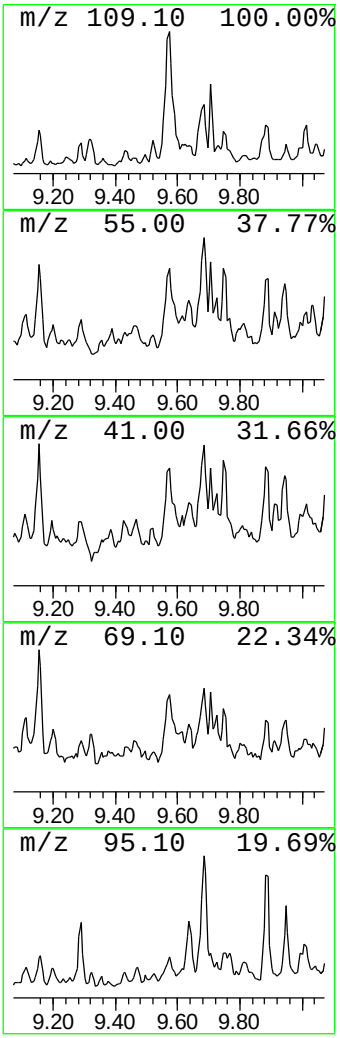
**********

Peak Number 6 2-[5-(2-Hydroxy-propyl)-fur... Concentration Rank 19

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.57 | 7.15 ng | 651031 | Acenaphthene-d10 | 10.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-[5-(2-Hydroxy-propyl)-furan-2-... | 184 | C10H16O3 | 1000187-25-5 | 50 |
| 2 | 6,6-Dimethylhepta-2,4-diene | 124 | C9H16 | 1000195-03-3 | 49 |
| 3 | Cyclohexanol, 3,3,5-trimethyl-, ... | 184 | C11H20O2 | 024691-16-5 | 47 |
| 4 | N-Cyclopropyl-p-fluorobenzylamine | 165 | C10H12FN | 1000250-88-9 | 43 |
| 5 | Ketone, isopropylidenecyclopropy... | 124 | C8H12O | 029765-67-1 | 43 |



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Data File : BF106422.D
Acq On : 14 Jun 2018 5:43
Operator : JU/SJ
Sample : J3398-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** W-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

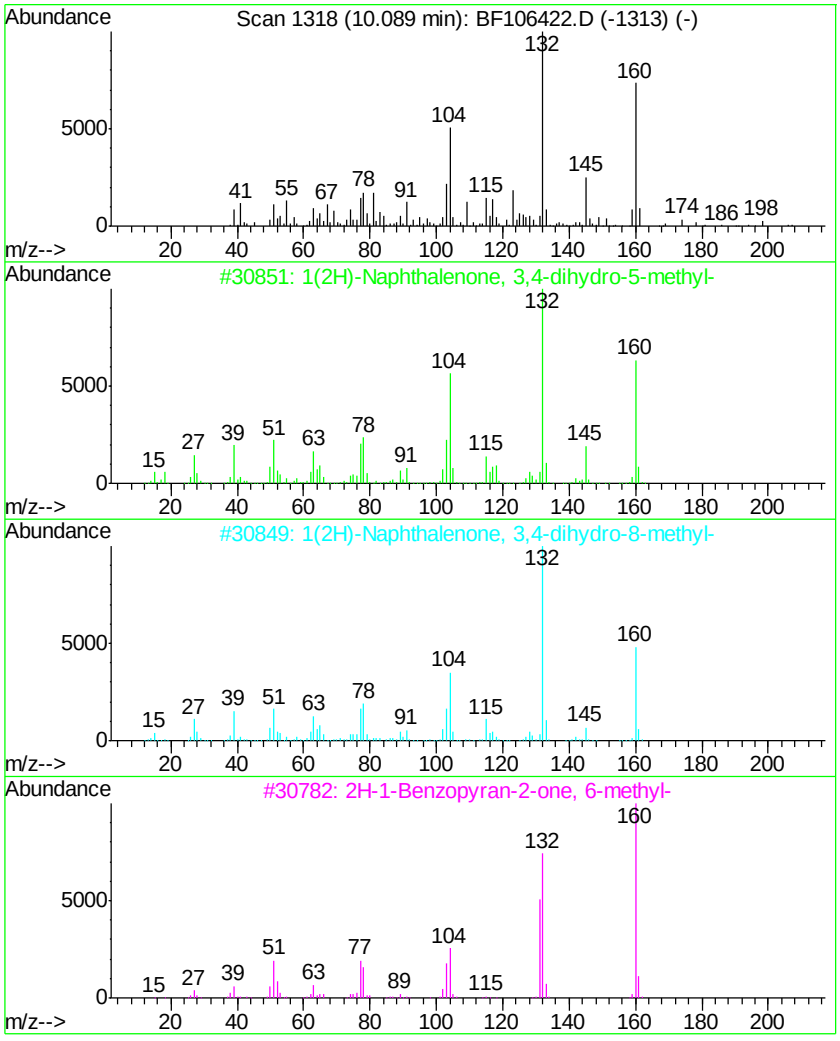
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

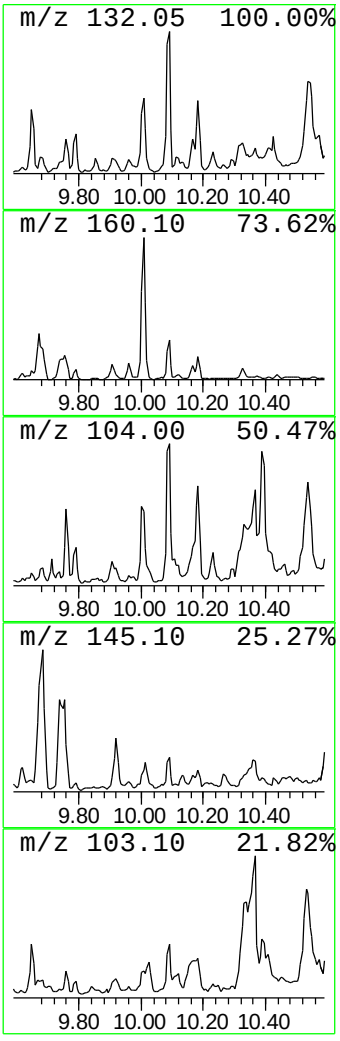
**********

Peak Number 7 1(2H)-Naphthalenone, 3,4-di... Concentration Rank 20

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.09 | 6.67 ng | 607253 | Acenaphthene-d10 | 10.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1(2H)-Naphthalenone, 3,4-dihydro... | 160 | C11H12O | 006939-35-1 | 91 |
| 2 | 1(2H)-Naphthalenone, 3,4-dihydro... | 160 | C11H12O | 051015-28-2 | 62 |
| 3 | 2H-1-Benzopyran-2-one, 6-methyl- | 160 | C10H8O2 | 000092-48-8 | 53 |
| 4 | 2-Methyl-1(2H)-phthalazinone | 160 | C9H8N2O | 006091-81-2 | 52 |
| 5 | 1-Benzosuberone | 160 | C11H12O | 000826-73-3 | 49 |



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Data File : BF106422.D
Acq On : 14 Jun 2018 5:43
Operator : JU/SJ
Sample : J3398-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** W-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

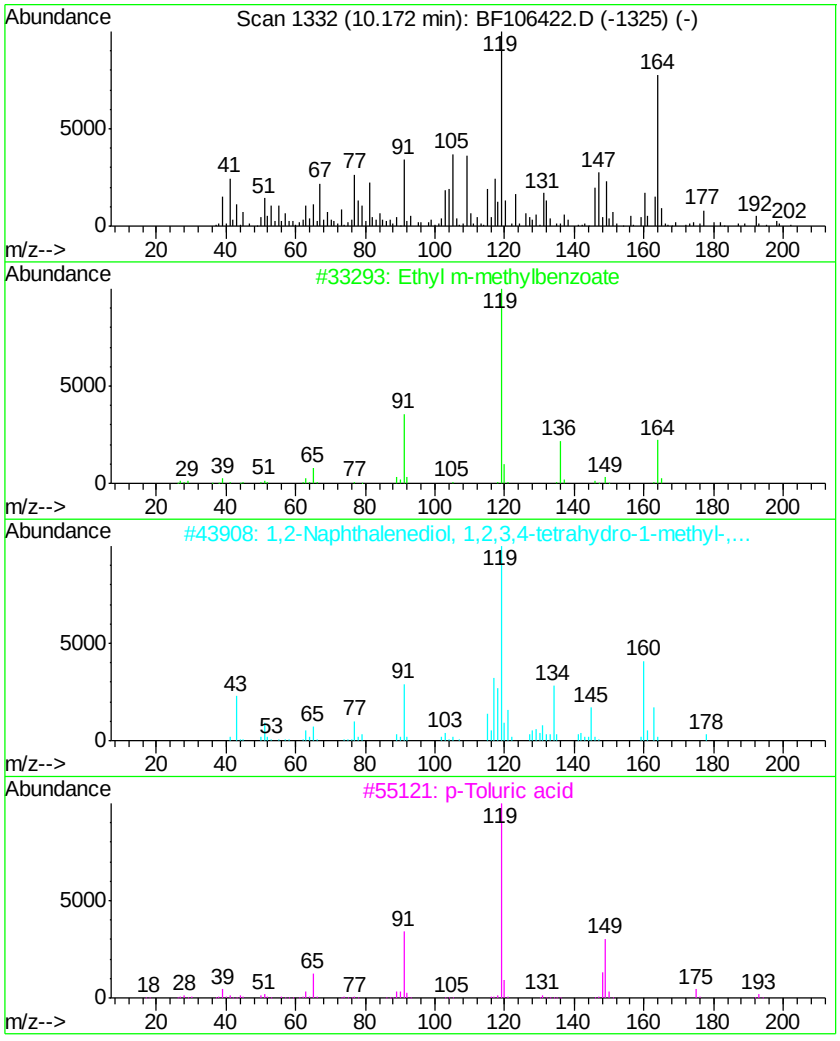
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

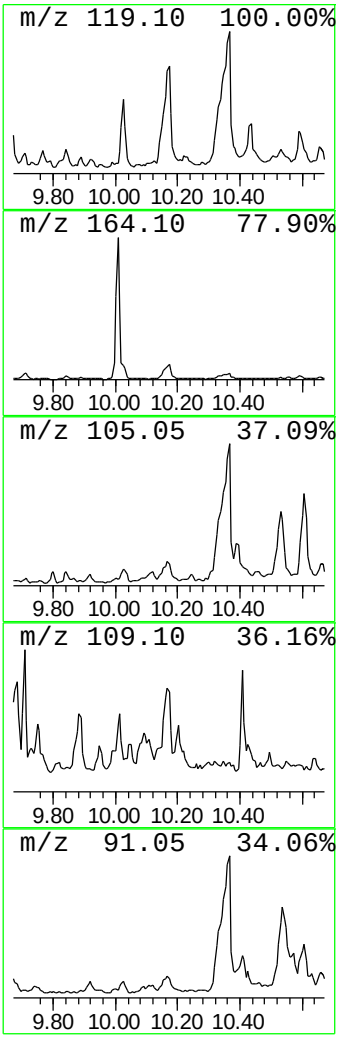
**********

Peak Number 8 unknown10.17 Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.17 | 10.25 ng | 933646 | Acenaphthene-d10 | 10.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethyl m-methylbenzoate | 164 | C10H12O2 | 000120-33-2 | 30 |
| 2 | 1,2-Naphthalenediol, 1,2,3,4-tet... | 178 | C11H14O2 | 056588-36-4 | 30 |
| 3 | p-Toluric acid | 193 | C10H11NO3 | 027115-50-0 | 20 |
| 4 | 7-Benzofuranol, 2,3-dihydro-2,2-... | 164 | C10H12O2 | 001563-38-8 | 20 |
| 5 | Benzonitrile, 3-ethoxy- | 147 | C9H9NO | 025117-75-3 | 18 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106422.D
Acq On : 14 Jun 2018 5:43
Operator : JU/SJ
Sample : J3398-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** W-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

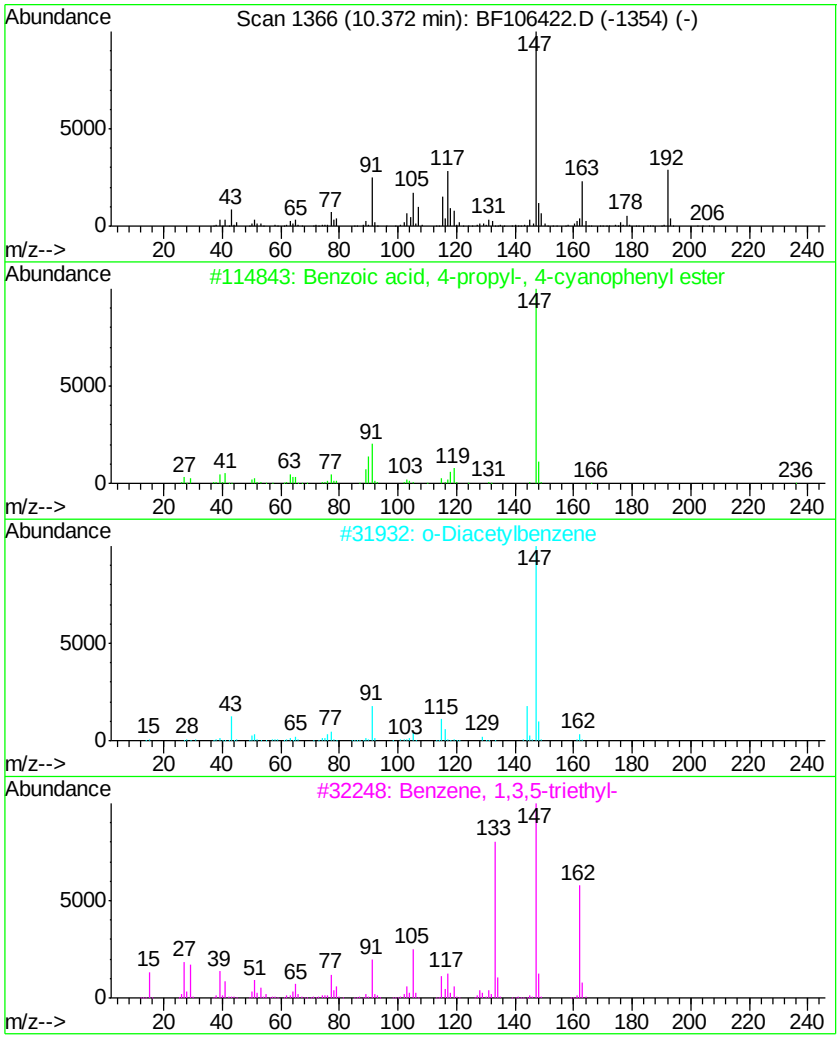
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

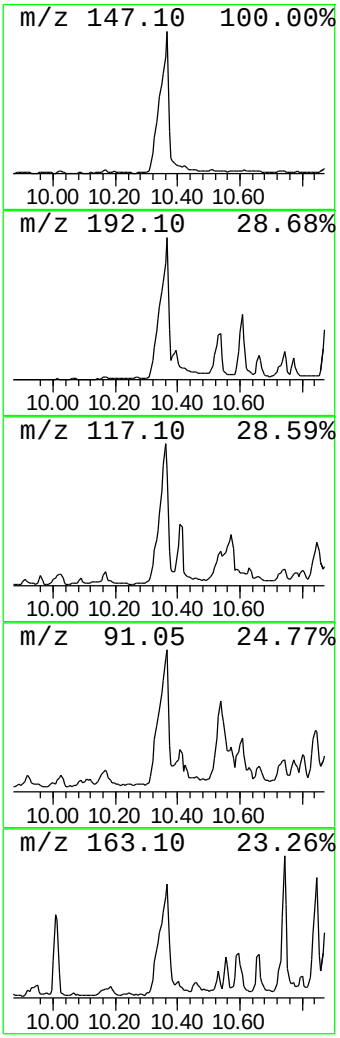
**********

Peak Number 9 unknown10.37 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.37 | 62.41 ng | 5685540 | Acenaphthene-d10 | 10.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzoic acid, 4-propyl-, 4-cyano... | 265 | C17H15NO2 | 056131-49-8 | 43 |
| 2 | o-Diacetylbenzene | 162 | C10H10O2 | 000704-00-7 | 43 |
| 3 | Benzene, 1,3,5-triethyl- | 162 | C12H18 | 000102-25-0 | 40 |
| 4 | 1H-Indazol-5-amine, 3-methyl- | 147 | C8H9N3 | 1000338-20-2 | 40 |
| 5 | Ethanone, 1-(2,4,5-trimethylphen... | 162 | C11H14O | 002040-07-5 | 38 |



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Data File : BF106422.D
Acq On : 14 Jun 2018 5:43
Operator : JU/SJ
Sample : J3398-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** W-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

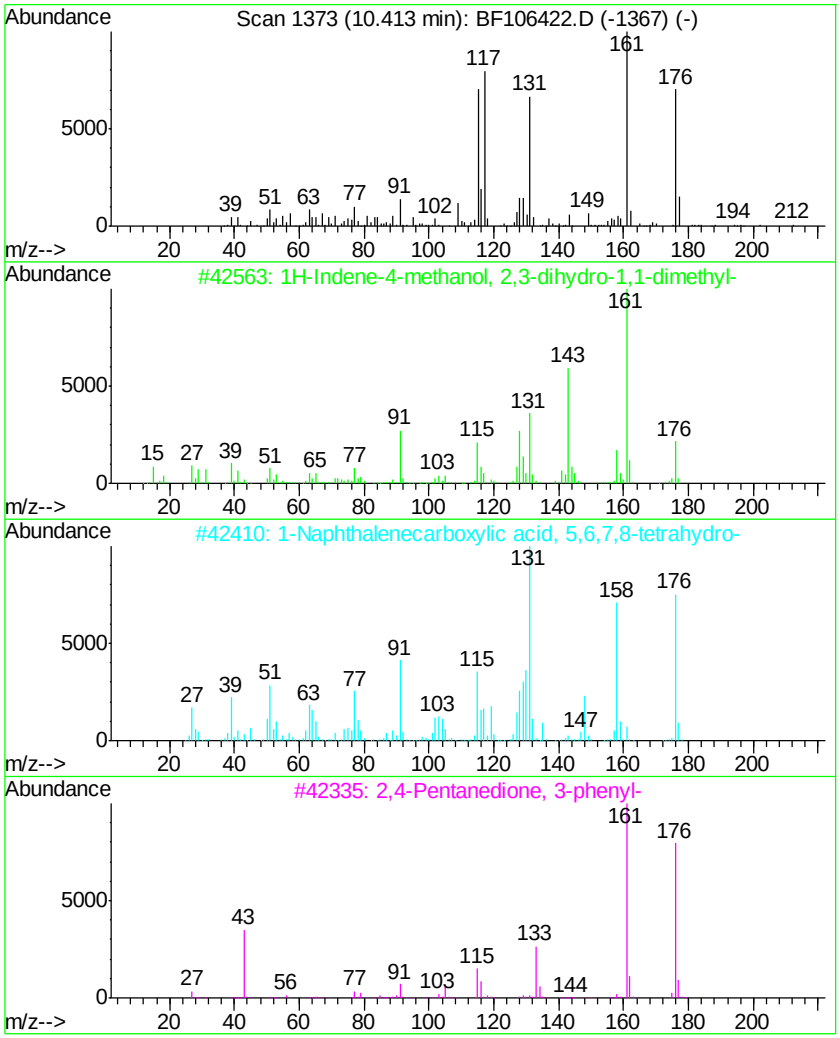
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

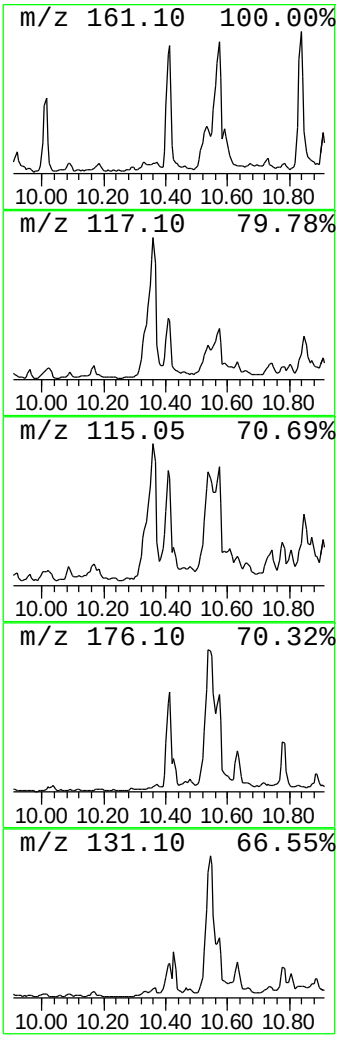
**********

Peak Number 10 1H-Indene-4-methanol, 2,3-d... Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.41 | 17.14 ng | 1561460 | Acenaphthene-d10 | 10.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1H-Indene-4-methanol, 2,3-dihydr... | 176 | C12H16O | 055591-09-8 | 53 |
| 2 | 1-Naphthalenecarboxylic acid, 5,... | 176 | C11H12O2 | 004242-18-6 | 38 |
| 3 | 2,4-Pentanedione, 3-phenyl- | 176 | C11H12O2 | 005910-25-8 | 27 |
| 4 | Benzofuran, 2,3-dihydro-2,2,4,6-... | 176 | C12H16O | 003698-49-5 | 25 |
| 5 | p-n-Butylacetophenone | 176 | C12H16O | 037920-25-5 | 25 |



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Data File : BF106422.D
Acq On : 14 Jun 2018 5:43
Operator : JU/SJ
Sample : J3398-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** W-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

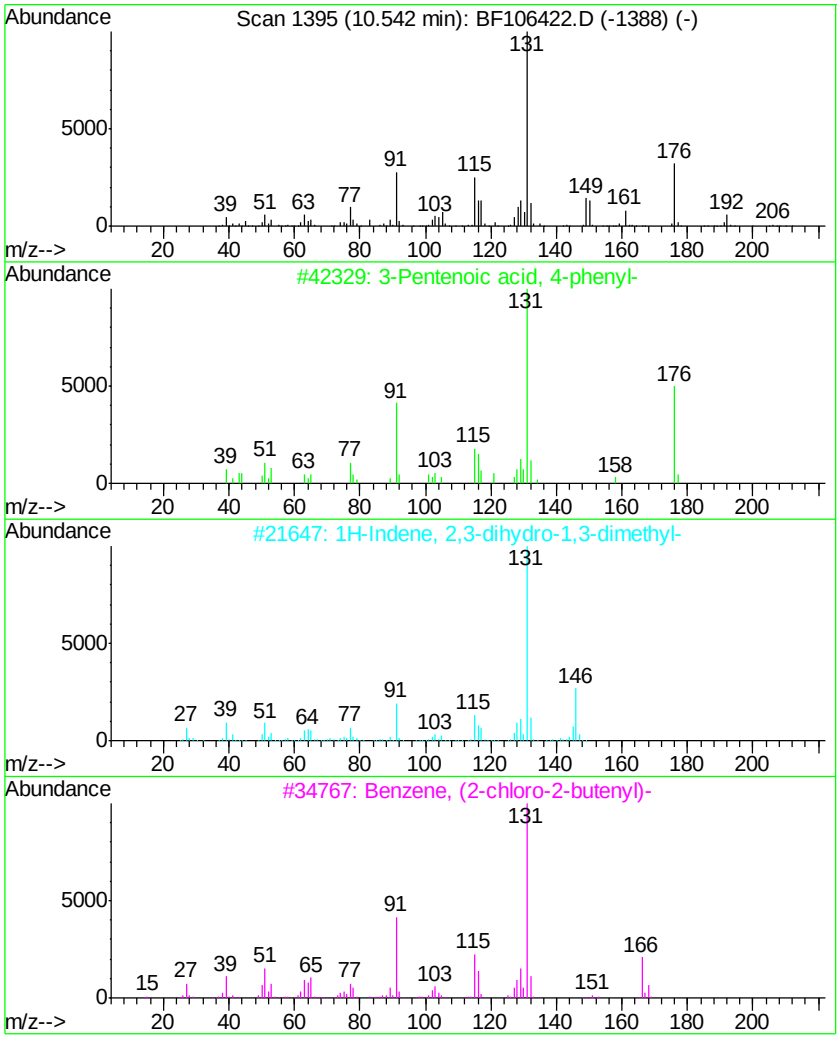
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

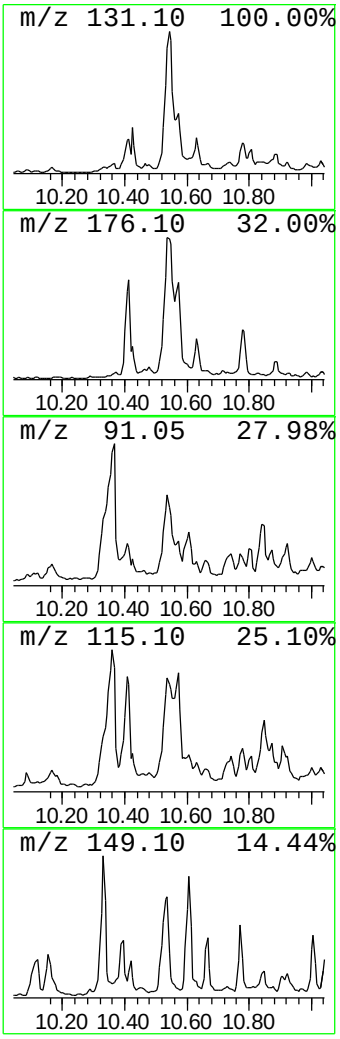
**********

Peak Number 11 3-Pentenoic acid, 4-phenyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.54 | 36.91 ng | 3362980 | Acenaphthene-d10 | 10.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Pentenoic acid, 4-phenyl- | 176 | C11H12O2 | 053774-19-9 | 60 |
| 2 | 1H-Indene, 2,3-dihydro-1,3-dimet... | 146 | C11H14 | 004175-53-5 | 43 |
| 3 | Benzene, (2-chloro-2-butenyl)- | 166 | C10H11Cl | 054411-12-0 | 43 |
| 4 | 1H-Indene, 2,3-dihydro-1,2-dimet... | 146 | C11H14 | 017057-82-8 | 43 |
| 5 | 1H-Indole, 1-methyl- | 131 | C9H9N | 000603-76-9 | 41 |



# Library Search Compound Report

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Data File : BF106422.D
Acq On : 14 Jun 2018 5:43
Operator : JU/SJ
Sample : J3398-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** W-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

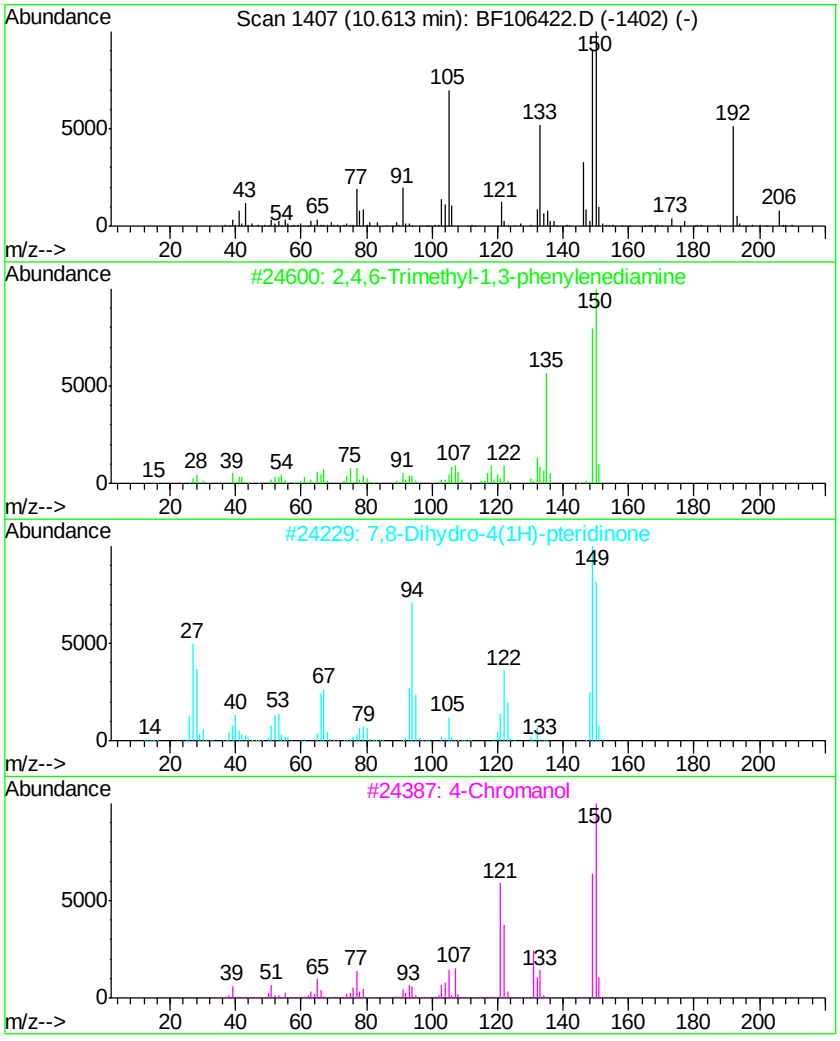
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

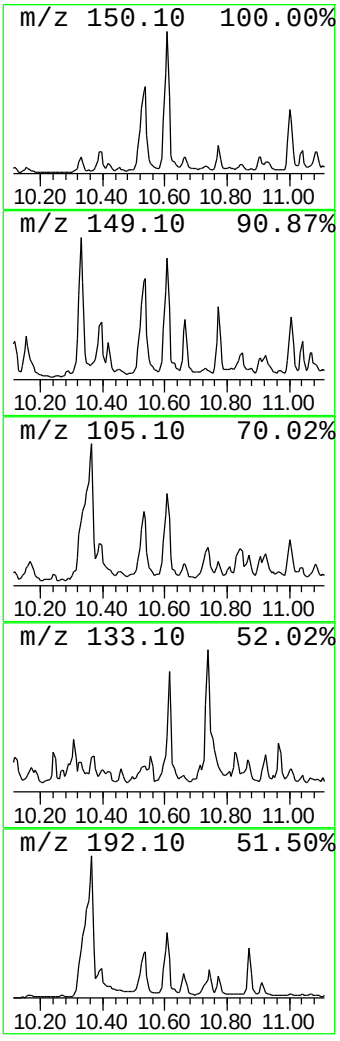
**********

Peak Number 12 2,4,6-Trimethyl-1,3-phenyle... Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.61 | 15.05 ng | 1370670 | Acenaphthene-d10 | 10.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,4,6-Trimethyl-1,3-phenylenedia... | 150 | C9H14N2 | 003102-70-3 | 53 |
| 2 | 7,8-Dihydro-4(1H)-pteridinone | 150 | C6H6N4O | 089418-07-5 | 53 |
| 3 | 4-Chromanol | 150 | C9H10O2 | 001481-93-2 | 53 |
| 4 | 2-Methoxy-5-methylbenzaldehyde | 150 | C9H10O2 | 007083-19-4 | 53 |
| 5 | 4-Pyridinamine, N,N,2,6-tetramet... | 150 | C9H14N2 | 129384-12-9 | 50 |



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Data File : BF106422.D
Acq On : 14 Jun 2018 5:43
Operator : JU/SJ
Sample : J3398-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** W-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

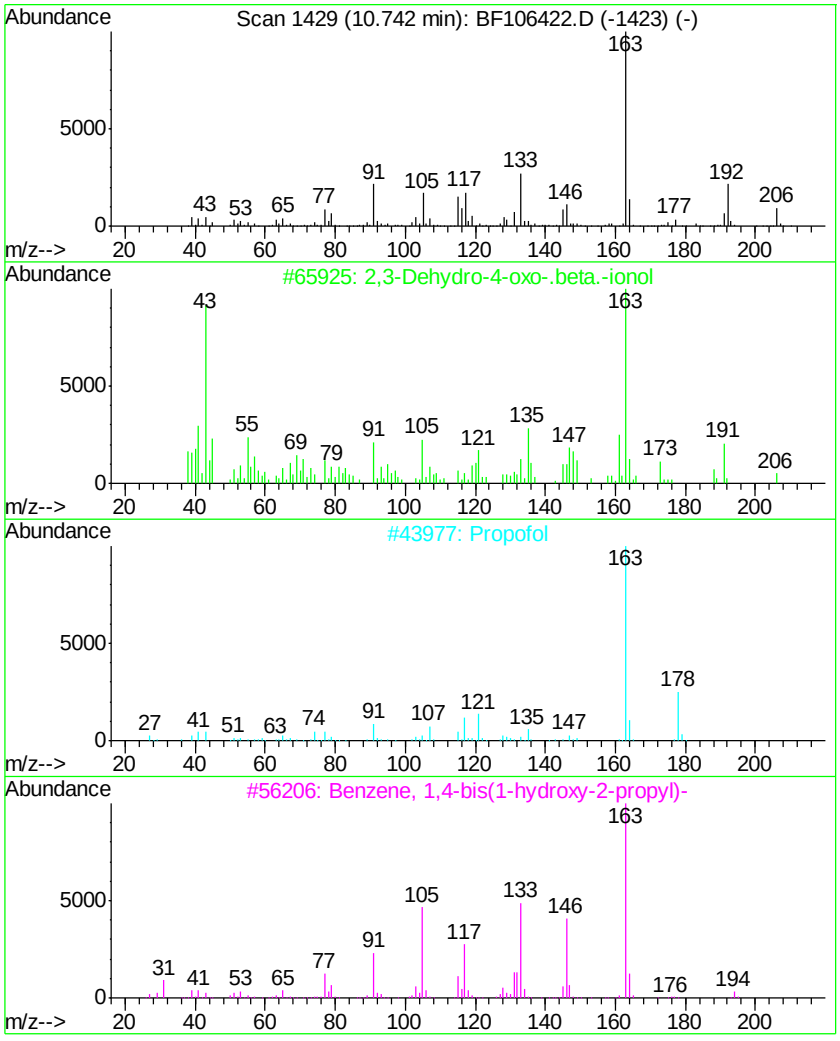
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

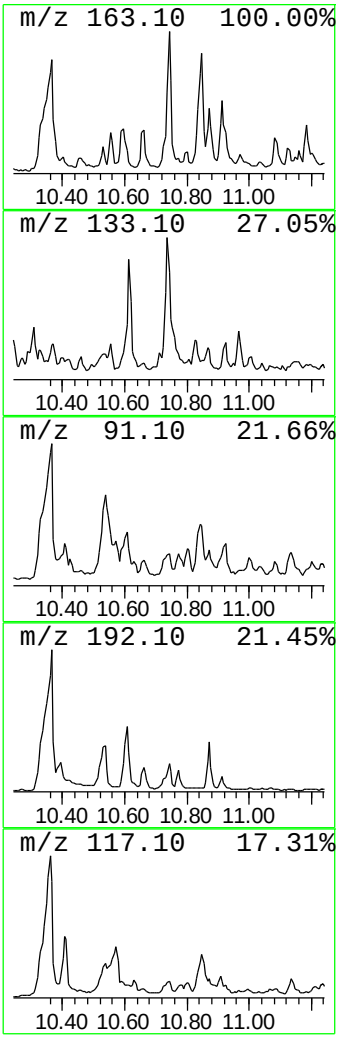
**********

Peak Number 13 2,3-Dehydro-4-oxo-.beta.-ionol Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.74 | 9.91 ng | 902786 | Acenaphthene-d10 | 10.01 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,3-Dehydro-4-oxo-.beta.-ionol | 206 | C13H18O2 | 1000108-72-3 | 50 |
| 2 | Propofol | 178 | C12H18O | 002078-54-8 | 43 |
| 3 | Benzene, 1,4-bis(1-hydroxy-2-pro... | 194 | C12H18O2 | 1000161-06-4 | 40 |
| 4 | p-Allylnitrobenzene | 163 | C9H9NO2 | 053483-17-3 | 38 |
| 5 | Benzoic acid, p-tert-butyl- | 178 | C11H14O2 | 000098-73-7 | 38 |



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Data File : BF106422.D
Acq On : 14 Jun 2018 5:43
Operator : JU/SJ
Sample : J3398-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** W-15

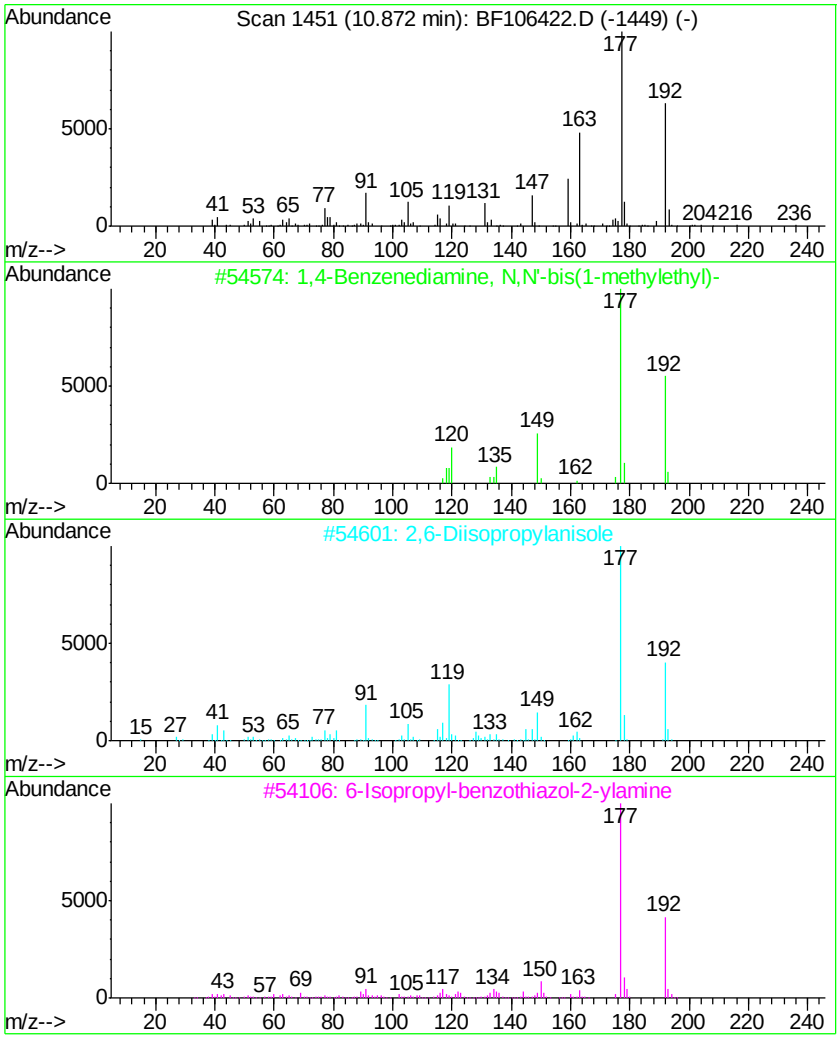
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

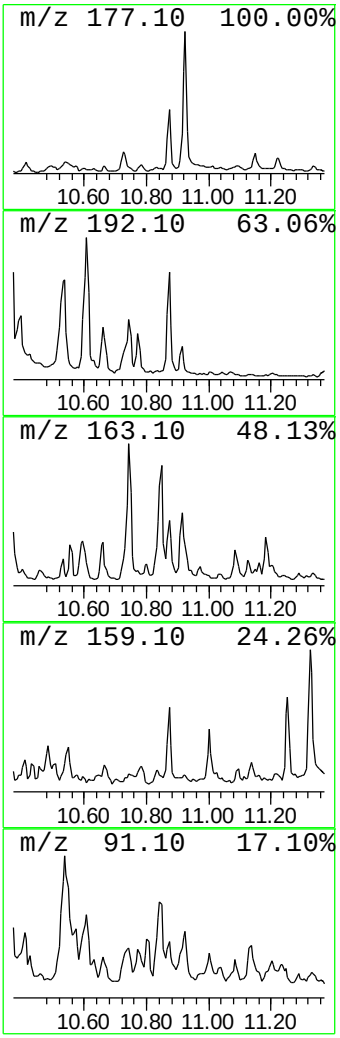
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 14 1,4-Benzenediamine, N,N'-bi... Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.87 | 10.69 ng | 646346 | Phenanthrene-d10 | 11.50 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,4-Benzenediamine, N,N'-bis(1-m... | 192 | C12H20N2 | 004251-01-8 | 52 |
| 2 | 2,6-Diisopropylanisole | 192 | C13H20O | 002944-52-7 | 52 |
| 3 | 6-Isopropyl-benzothiazol-2-ylamine | 192 | C10H12N2S | 032895-14-0 | 47 |
| 4 | 2-Buten-1-one, 1-(2,6,6-trimethy... | 192 | C13H20O | 035044-68-9 | 47 |
| 5 | 1-(4-Methoxymethyl-2,6-dimethylp... | 192 | C12H16O2 | 1000202-02-2 | 46 |



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Data File : BF106422.D
Acq On : 14 Jun 2018 5:43
Operator : JU/SJ
Sample : J3398-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** W-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

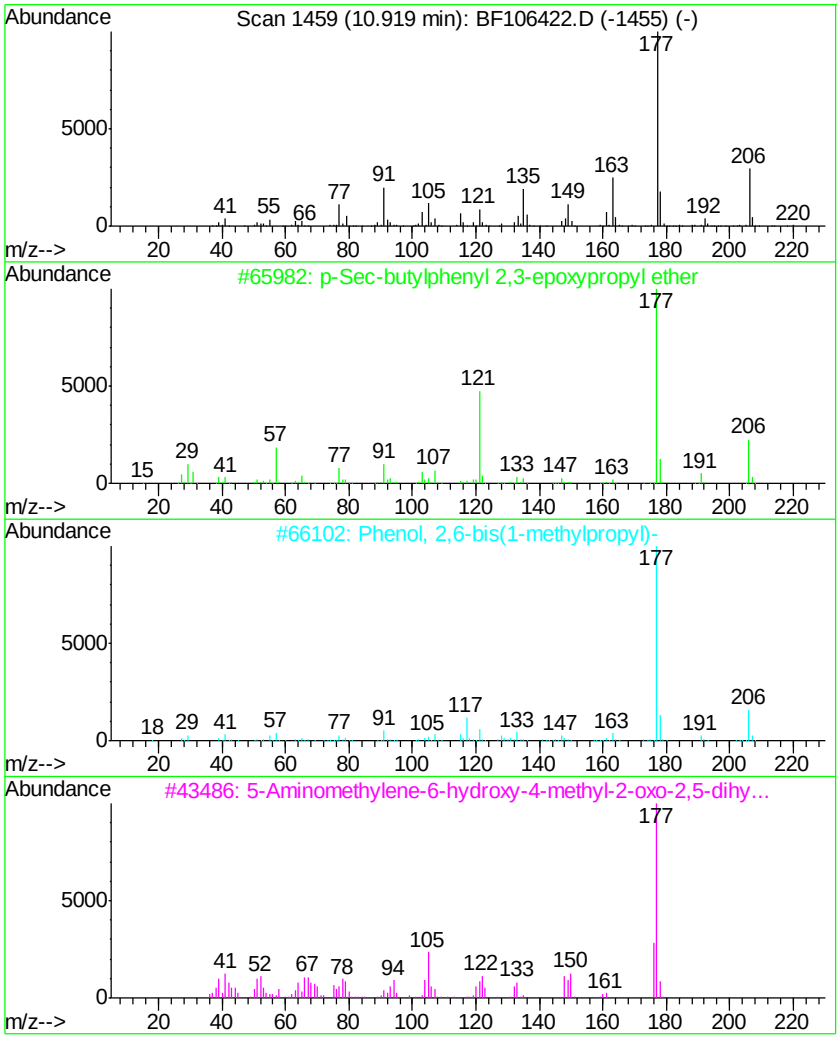
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

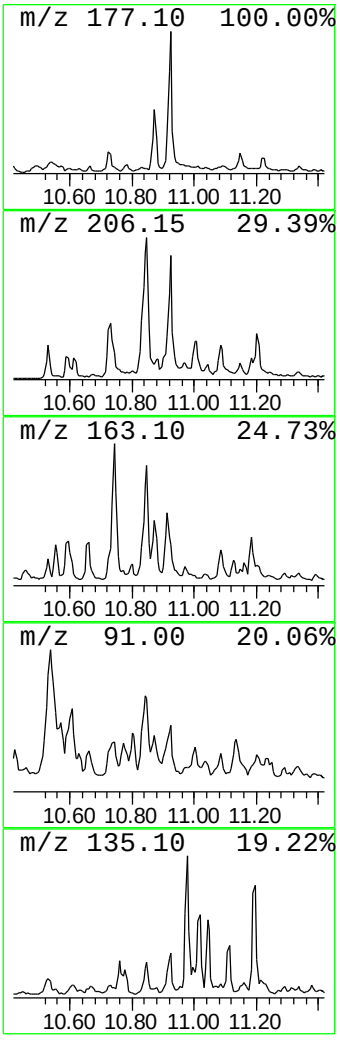
**********

Peak Number 15 p-Sec-butylphenyl 2,3-epoxy... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.92 | 19.89 ng | 1202730 | Phenanthrene-d10 | 11.50 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | p-Sec-butylphenyl 2,3-epoxypropy... | 206 | C13H18O2 | 067557-76-0 | 62 |
| 2 | Phenol, 2,6-bis(1-methylpropyl)- | 206 | C14H22O | 005510-99-6 | 58 |
| 3 | 5-Aminomethylene-6-hydroxy-4-met... | 177 | C8H7N3O2 | 1000223-27-4 | 50 |
| 4 | trans-.beta.-Ionone | 192 | C13H20O | 000079-77-6 | 42 |
| 5 | 1,3-di-n-Propyladamantane | 220 | C16H28 | 040002-47-9 | 42 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106422.D
Acq On : 14 Jun 2018 5:43
Operator : JU/SJ
Sample : J3398-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** W-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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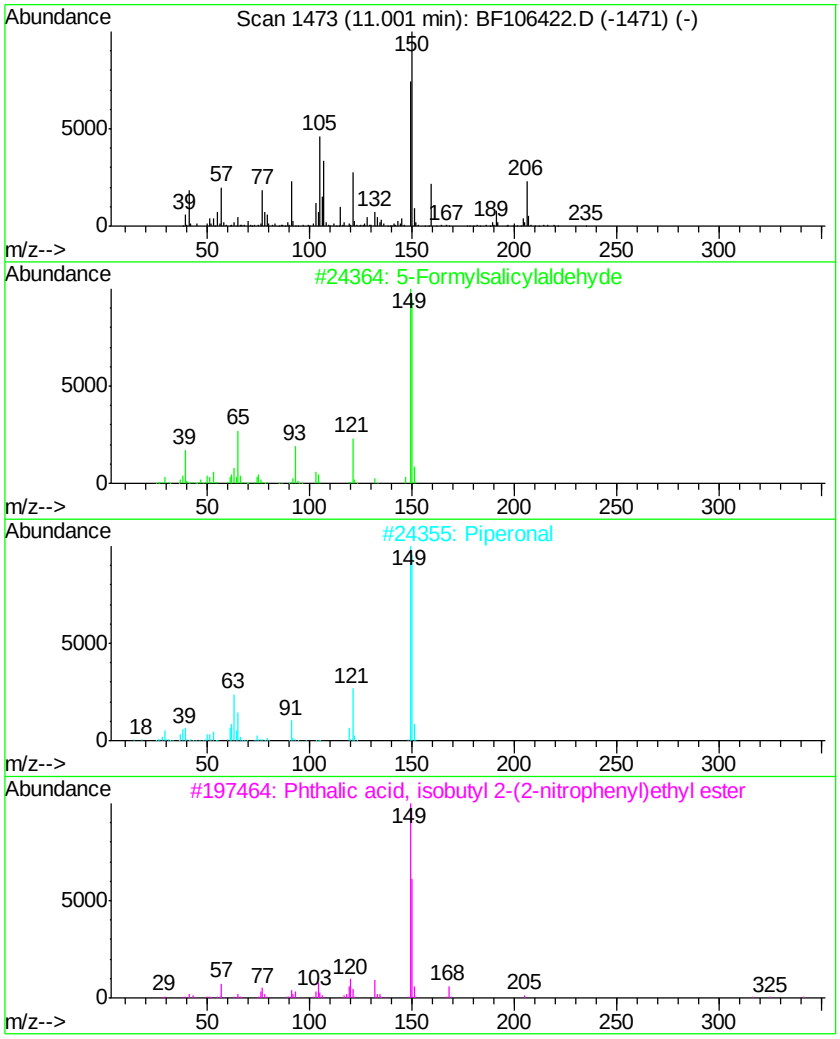
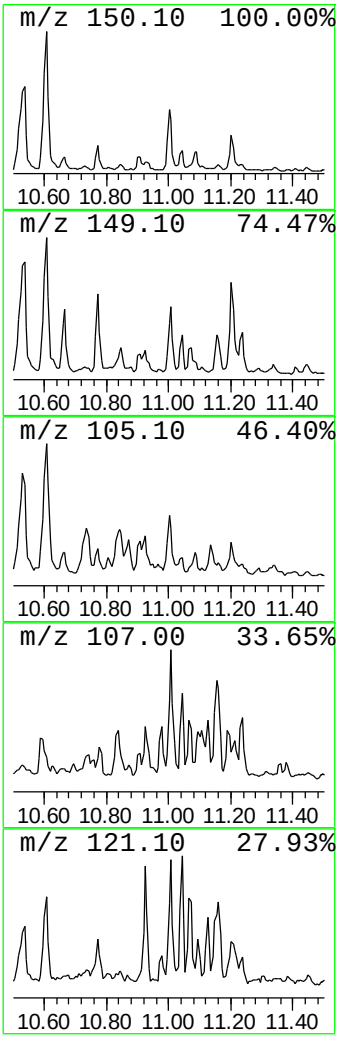
Peak Number 16 5-Formylsalicylaldehyde Concentration Rank 18

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.00 | 7.21 ng | 435692 | Phenanthrene-d10 | 11.50 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Formylsalicylaldehyde | 150 | C8H6O3 | 003328-70-9 | 50 |
| 2 | Piperonal | 150 | C8H6O3 | 000120-57-0 | 40 |
| 3 | Phthalic acid, isobutyl 2-(2-nit... | 371 | C20H21NO6 | 1000377-99-3 | 32 |
| 4 | 2-Hydroxy-4,6-dimethylbenzaldehyde | 150 | C9H10O2 | 001666-02-0 | 32 |
| 5 | Benzoic acid, 3,5-dimethyl- | 150 | C9H10O2 | 000499-06-9 | 30 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106422.D
Acq On : 14 Jun 2018 5:43
Operator : JU/SJ
Sample : J3398-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** W-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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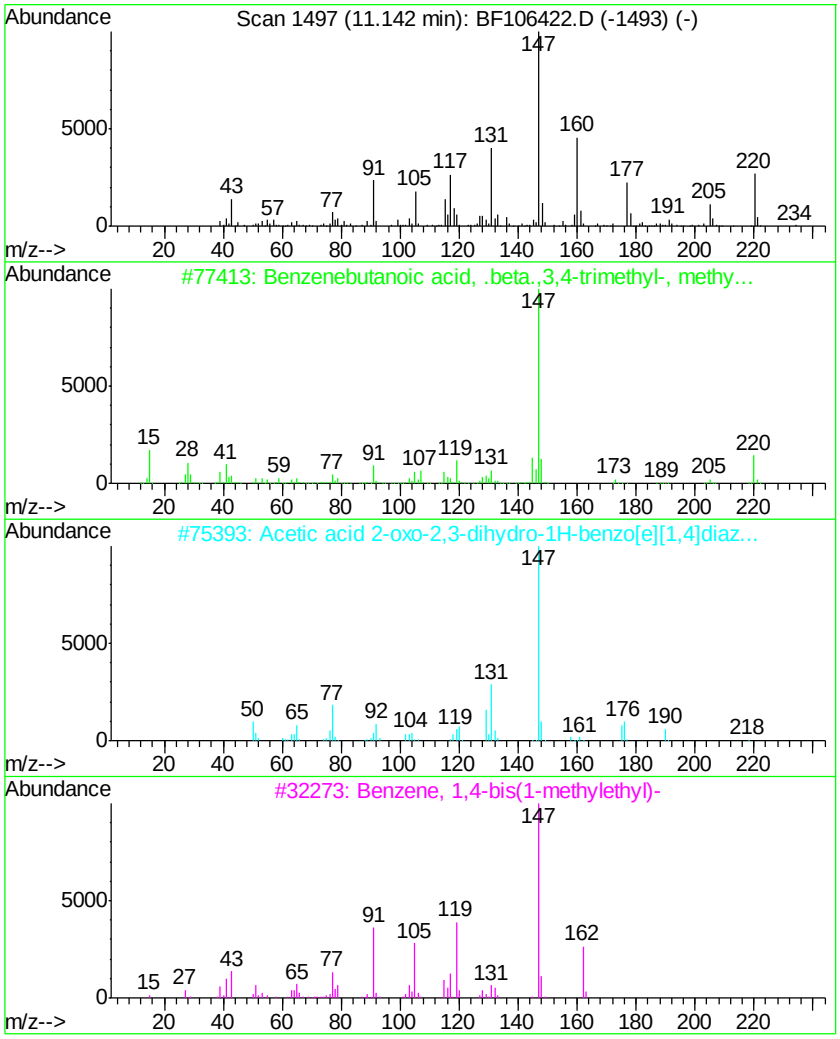
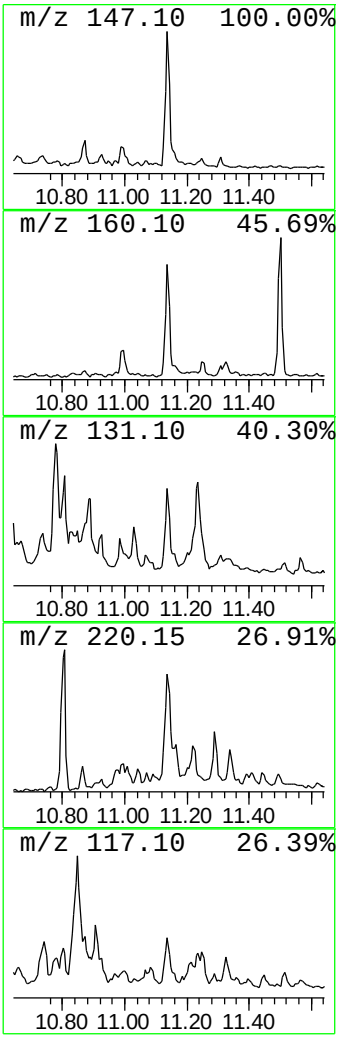
Peak Number 17 unknown11.14 Concentration Rank 15

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.14 | 9.79 ng | 592045 | Phenanthrene-d10 | 11.50 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzenebutanoic acid, .beta.,3,4... | 220 | C14H20O2 | 069855-51-2 | 38 |
| 2 | Acetic acid 2-oxo-2,3-dihydro-1H... | 218 | C11H10N2O3 | 016780-58-8 | 37 |
| 3 | Benzene, 1,4-bis(1-methylethyl)- | 162 | C12H18 | 000100-18-5 | 35 |
| 4 | Benzene, 1,2-diethyl-3,4-dimethyl- | 162 | C12H18 | 054410-75-2 | 30 |
| 5 | Benzoic acid, 4-propyl-, 4-cyano... | 265 | C17H15NO2 | 056131-49-8 | 27 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106422.D
Acq On : 14 Jun 2018 5:43
Operator : JU/SJ
Sample : J3398-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** W-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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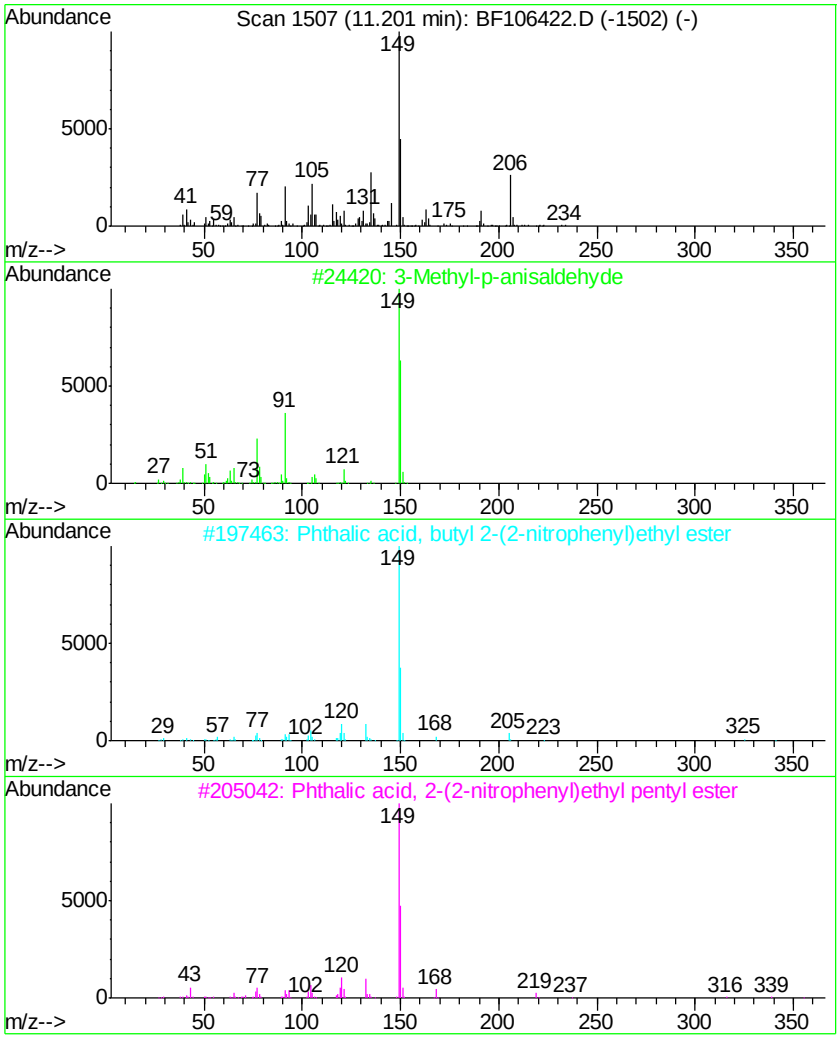
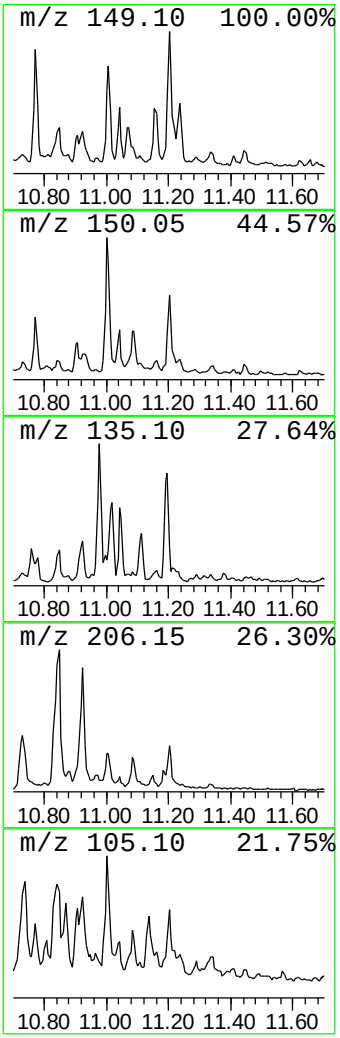
Peak Number 18 unknown11.20 Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.20 | 13.50 ng | 816215 | Phenanthrene-d10 | 11.50 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Methyl-p-anisaldehyde | 150 | C9H10O2 | 032723-67-4 | 46 |
| 2 | Phthalic acid, butyl 2-(2-nitrop... | 371 | C20H21NO6 | 1000377-99-4 | 43 |
| 3 | Phthalic acid, 2-(2-nitrophenyl)... | 385 | C21H23NO6 | 1000377-99-5 | 43 |
| 4 | Benzenepropanoic acid, .alpha.-(... | 206 | C13H18O2 | 053483-12-8 | 40 |
| 5 | 2-t-Butyl-6-[2-hydroxy-2-(2,4,6-... | 318 | C19H26O4 | 1000192-88-0 | 38 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106422.D
Acq On : 14 Jun 2018 5:43
Operator : JU/SJ
Sample : J3398-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** W-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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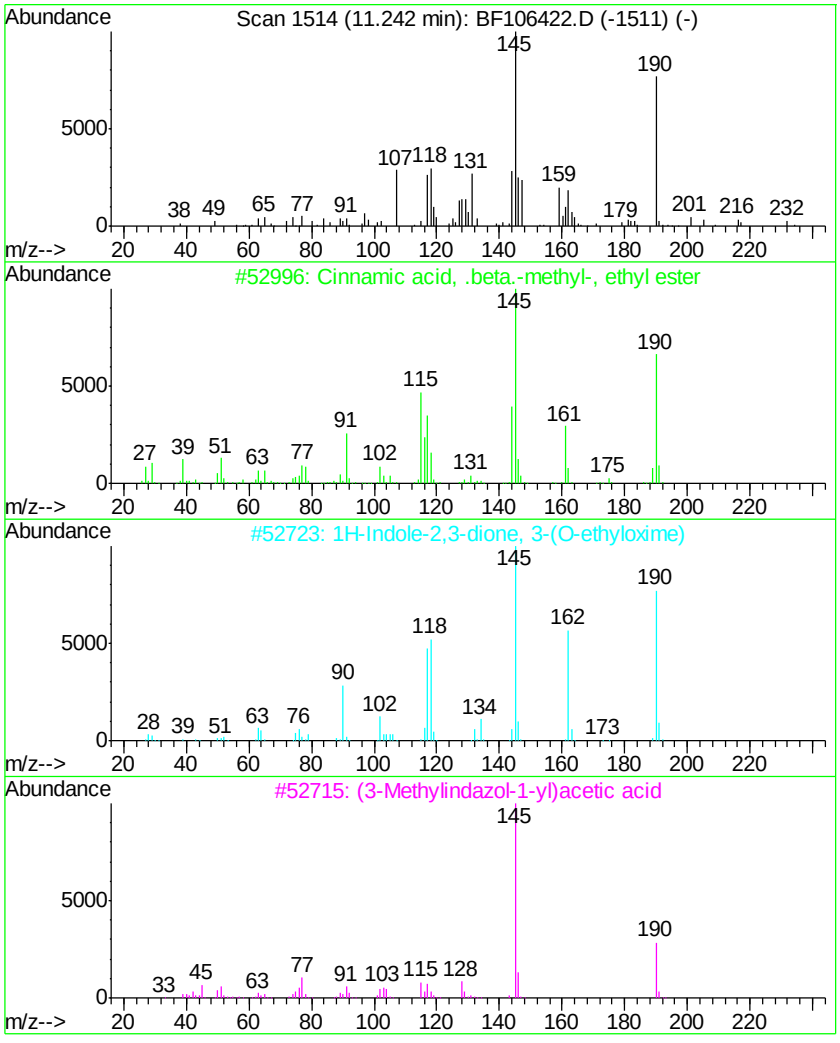
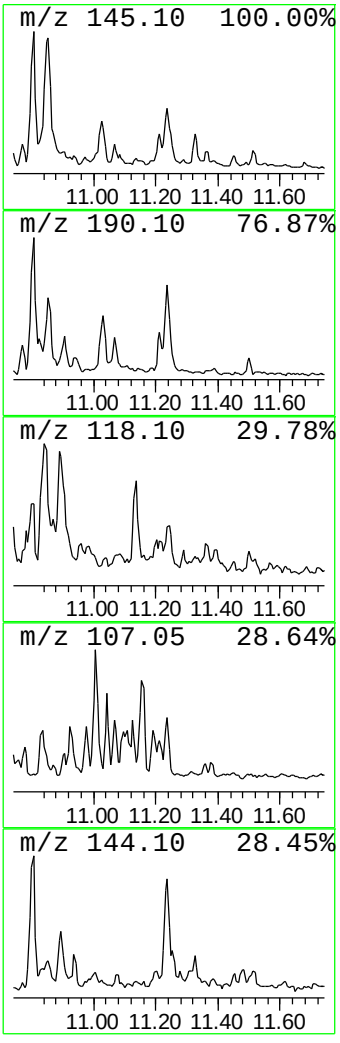
Peak Number 19 unknown11.24 Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.24 | 10.17 ng | 614644 | Phenanthrene-d10 | 11.50 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cinnamic acid, .beta.-methyl-, e... | 190 | C12H14O2 | 000945-93-7 | 41 |
| 2 | 1H-Indole-2,3-dione, 3-(O-ethylo... | 190 | C10H10N2O2 | 1000349-79-7 | 22 |
| 3 | (3-Methylindazol-1-yl)acetic acid | 190 | C10H10N2O2 | 1000316-00-6 | 22 |
| 4 | Phenylthio 2-benzylpent-3-enoate | 282 | C18H18OS | 1000284-46-0 | 14 |
| 5 | 2-Propenoic acid, 3-(4-methylphe... | 190 | C12H14O2 | 020511-20-0 | 12 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106422.D
Acq On : 14 Jun 2018 5:43
Operator : JU/SJ
Sample : J3398-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** W-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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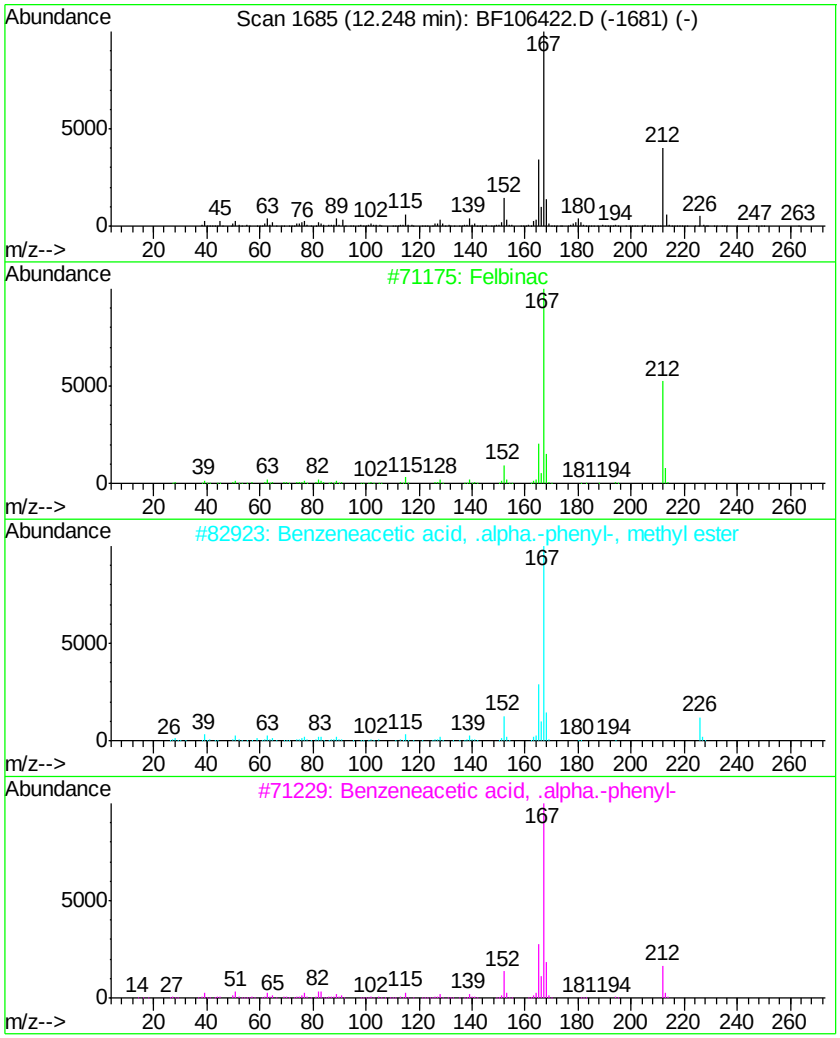
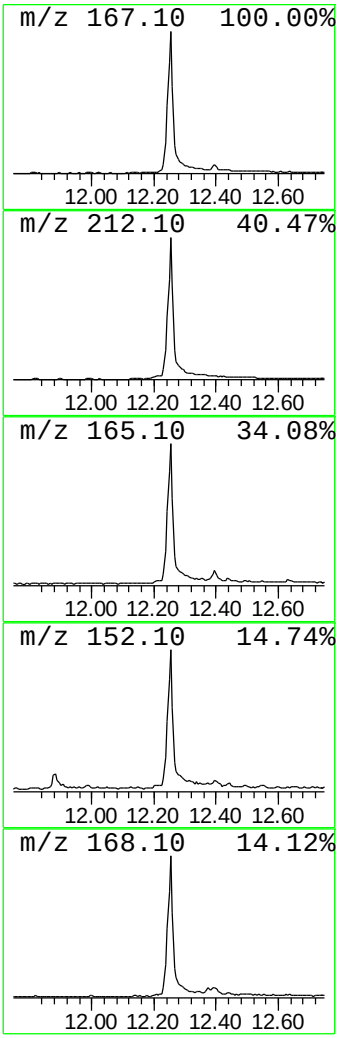
Peak Number 20 Felbinac Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.25 | 25.46 ng | 1539180 | Phenanthrene-d10 | 11.50 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Felbinac | 212 | C14H12O2 | 005728-52-9 | 94 |
| 2 | Benzeneacetic acid, .alpha.-phen... | 226 | C15H14O2 | 003469-00-9 | 89 |
| 3 | Benzeneacetic acid, .alpha.-phenyl- | 212 | C14H12O2 | 000117-34-0 | 87 |
| 4 | 1,1'-Biphenyl, 4-(chloromethyl)- | 202 | C13H11Cl | 001667-11-4 | 70 |
| 5 | Benzeneacetaldehyde, .alpha.-phe... | 196 | C14H12O | 000947-91-1 | 68 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061318\
Data File : BF106422.D
Acq On : 14 Jun 2018 5:43
Operator : JU/SJ
Sample : J3398-05
Misc :
ALS Vial : 35 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** W-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| unknown6.75 | 6.75 | 62.0 | ng | 2787990 | 1 | 6.97 | 899956 | 20.0 |
| Indane | 7.14 | 7.4 | ng | 331719 | 1 | 6.97 | 899956 | 20.0 |
| Benzene, 1,2,4,5-... | 7.98 | 21.5 | ng | 1431460 | 2 | 8.25 | 1333210 | 20.0 |
| Naphthalene, 1-me... | 9.06 | 8.2 | ng | 546651 | 2 | 8.25 | 1333210 | 20.0 |
| 2-[5-(2-Hydroxy-p... | 9.57 | 7.2 | ng | 651031 | 3 | 10.01 | 1822030 | 20.0 |
| 1(2H)-Naphthaleno... | 10.09 | 6.7 | ng | 607253 | 3 | 10.01 | 1822030 | 20.0 |
| unknown10.17 | 10.17 | 10.3 | ng | 933646 | 3 | 10.01 | 1822030 | 20.0 |
| unknown10.37 | 10.37 | 62.4 | ng | 5685540 | 3 | 10.01 | 1822030 | 20.0 |
| 1H-Indene-4-metha... | 10.41 | 17.1 | ng | 1561460 | 3 | 10.01 | 1822030 | 20.0 |
| 3-Pentenoic acid,... | 10.54 | 36.9 | ng | 3362980 | 3 | 10.01 | 1822030 | 20.0 |
| 2,4,6-Trimethyl-1... | 10.61 | 15.1 | ng | 1370670 | 3 | 10.01 | 1822030 | 20.0 |
| 2,3-Dehydro-4-oxo... | 10.74 | 9.9 | ng | 902786 | 3 | 10.01 | 1822030 | 20.0 |
| 1,4-Benzenediamin... | 10.87 | 10.7 | ng | 646346 | 4 | 11.50 | 1209300 | 20.0 |
| p-Sec-butylphenyl... | 10.92 | 19.9 | ng | 1202730 | 4 | 11.50 | 1209300 | 20.0 |
| 5-Formylsalicylal... | 11.00 | 7.2 | ng | 435692 | 4 | 11.50 | 1209300 | 20.0 |
| unknown11.14 | 11.14 | 9.8 | ng | 592045 | 4 | 11.50 | 1209300 | 20.0 |
| unknown11.20 | 11.20 | 13.5 | ng | 816215 | 4 | 11.50 | 1209300 | 20.0 |
| unknown11.24 | 11.24 | 10.2 | ng | 614644 | 4 | 11.50 | 1209300 | 20.0 |
| Felbinac | 12.25 | 25.5 | ng | 1539180 | 4 | 11.50 | 1209300 | 20.0 |