LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080715\
Data File : BF080927.D
Acq On : 7 Aug 2015 15:20
Operator : TP/UM
Sample : G3083-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 8524

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080715.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 4.967 | 249 | 252 | 254 | rBV | 678882 | 920861 | 16.53% | 0.958% |
| 2 | 5.390 | 286 | 289 | 291 | rBV | 1224165 | 1201953 | 21.58% | 1.251% |
| 3 | 6.464 | 378 | 383 | 385 | rBV2 | 1653951 | 3177691 | 57.05% | 3.307% |
| 4 | 6.590 | 388 | 394 | 397 | rVV3 | 1629934 | 3790268 | 68.05% | 3.944% |
| 5 | 6.807 | 411 | 413 | 415 | rBV | 380864 | 302796 | 5.44% | 0.315% |
| 6 | 6.967 | 424 | 427 | 430 | rBV2 | 1007801 | 1536348 | 27.58% | 1.599% |
| 7 | 7.070 | 433 | 436 | 442 | rVB2 | 1030504 | 2637233 | 47.35% | 2.744% |
| 8 | 7.230 | 447 | 450 | 453 | rBV | 1151995 | 1473267 | 26.45% | 1.533% |
| 9 | 7.379 | 460 | 463 | 465 | rBV | 742283 | 908039 | 16.30% | 0.945% |
| 10 | 7.642 | 483 | 486 | 489 | rBV | 2142283 | 2628426 | 47.19% | 2.735% |
| 11 | 7.710 | 490 | 492 | 495 | rVB | 572183 | 589275 | 10.58% | 0.613% |
| 12 | 7.847 | 502 | 504 | 506 | rVB | 729554 | 693888 | 12.46% | 0.722% |
| 13 | 8.042 | 518 | 521 | 523 | rBV | 2025118 | 1944609 | 34.92% | 2.024% |
| 14 | 8.122 | 523 | 528 | 530 | rVB2 | 1880791 | 2137441 | 38.38% | 2.224% |
| 15 | 8.236 | 536 | 538 | 541 | rVB | 1202135 | 1150239 | 20.65% | 1.197% |
| 16 | 8.647 | 571 | 574 | 576 | rBV | 932997 | 1191182 | 21.39% | 1.240% |
| 17 | 8.807 | 585 | 588 | 591 | rBV | 1871518 | 2001878 | 35.94% | 2.083% |
| 18 | 9.082 | 609 | 612 | 614 | rBV | 1091591 | 1497811 | 26.89% | 1.559% |
| 19 | 9.127 | 614 | 616 | 618 | rVV | 1823680 | 2199878 | 39.50% | 2.289% |
| 20 | 9.173 | 618 | 620 | 622 | rVB | 1733633 | 1536771 | 27.59% | 1.599% |
| 21 | 9.299 | 628 | 631 | 633 | rVB | 2453544 | 2335301 | 41.93% | 2.430% |
| 22 | 9.585 | 653 | 656 | 657 | rBV | 39029 | 56903 | 1.02% | 0.059% |
| 23 | 9.642 | 657 | 661 | 663 | rVV | 1955113 | 2343114 | 42.07% | 2.438% |
| 24 | 9.710 | 664 | 667 | 669 | rBV | 1118811 | 1061998 | 19.07% | 1.105% |
| 25 | 9.847 | 676 | 679 | 681 | rBV | 549088 | 469249 | 8.43% | 0.488% |
| 26 | 10.065 | 693 | 698 | 700 | rVB2 | 3311054 | 5569544 | 100.00% | 5.796% |
| 27 | 10.396 | 724 | 727 | 729 | rVB | 3607491 | 3736868 | 67.09% | 3.889% |
| 28 | 10.625 | 745 | 747 | 750 | rVB2 | 780768 | 1055321 | 18.95% | 1.098% |
| 29 | 10.888 | 766 | 770 | 772 | rBV | 3208653 | 3674152 | 65.97% | 3.823% |
| 30 | 10.945 | 772 | 775 | 777 | rVB | 688787 | 731295 | 13.13% | 0.761% |
| 31 | 11.128 | 789 | 791 | 794 | rBV | 1055680 | 1264825 | 22.71% | 1.316% |
| 32 | 11.322 | 806 | 808 | 811 | rBV | 572921 | 498573 | 8.95% | 0.519% |
| 33 | 11.413 | 812 | 816 | 818 | rBV | 3212452 | 3640025 | 65.36% | 3.788% |
| 34 | 11.905 | 856 | 859 | 862 | rVB | 3451874 | 3961669 | 71.13% | 4.123% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080715\
Data File : BF080927.D
Acq On : 7 Aug 2015 15:20
Operator : TP/UM
Sample : G3083-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 8524

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080715.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 12.145 | 878 | 880 | 882 | rVB | 149543 | 145346 | 2.61% | 0.151% |
| 36 | 12.533 | 912 | 914 | 917 | rBV | 1326570 | 1276989 | 22.93% | 1.329% |
| 37 | 12.682 | 925 | 927 | 929 | rBV | 70358 | 57785 | 1.04% | 0.060% |
| 38 | 12.773 | 931 | 935 | 937 | rVV | 2999313 | 3757474 | 67.46% | 3.910% |
| 39 | 12.911 | 944 | 947 | 949 | rBV | 1968410 | 1871490 | 33.60% | 1.948% |
| 40 | 13.391 | 986 | 989 | 992 | rBV | 2602020 | 3106459 | 55.78% | 3.233% |
| 41 | 13.871 | 1028 | 1031 | 1035 | rBV3 | 32089 | 113957 | 2.05% | 0.119% |
| 42 | 13.951 | 1035 | 1038 | 1040 | rVV2 | 2070866 | 3524347 | 63.28% | 3.668% |
| 43 | 14.008 | 1040 | 1043 | 1045 | rVB | 2832001 | 4764377 | 85.54% | 4.958% |
| 44 | 14.557 | 1089 | 1091 | 1094 | rBV | 1299393 | 1421708 | 25.53% | 1.479% |
| 45 | 14.797 | 1110 | 1112 | 1115 | rVB | 148504 | 155431 | 2.79% | 0.162% |
| 46 | 14.979 | 1123 | 1128 | 1129 | rBV | 1648166 | 3391389 | 60.89% | 3.529% |
| 47 | 15.014 | 1129 | 1131 | 1133 | rVB | 2262886 | 2766703 | 49.68% | 2.879% |
| 48 | 15.311 | 1153 | 1157 | 1159 | rBV | 1132370 | 1498649 | 26.91% | 1.560% |
| 49 | 15.357 | 1159 | 1161 | 1164 | rVB | 285260 | 424424 | 7.62% | 0.442% |
| 50 | 16.740 | 1275 | 1282 | 1285 | rBV | 851619 | 2177321 | 39.09% | 2.266% |
| 51 | 17.151 | 1310 | 1318 | 1321 | rBV | 684552 | 1663206 | 29.86% | 1.731% |
| 52 | 19.163 | 1489 | 1494 | 1501 | rVB2 | 20948 | 59508 | 1.07% | 0.062% |

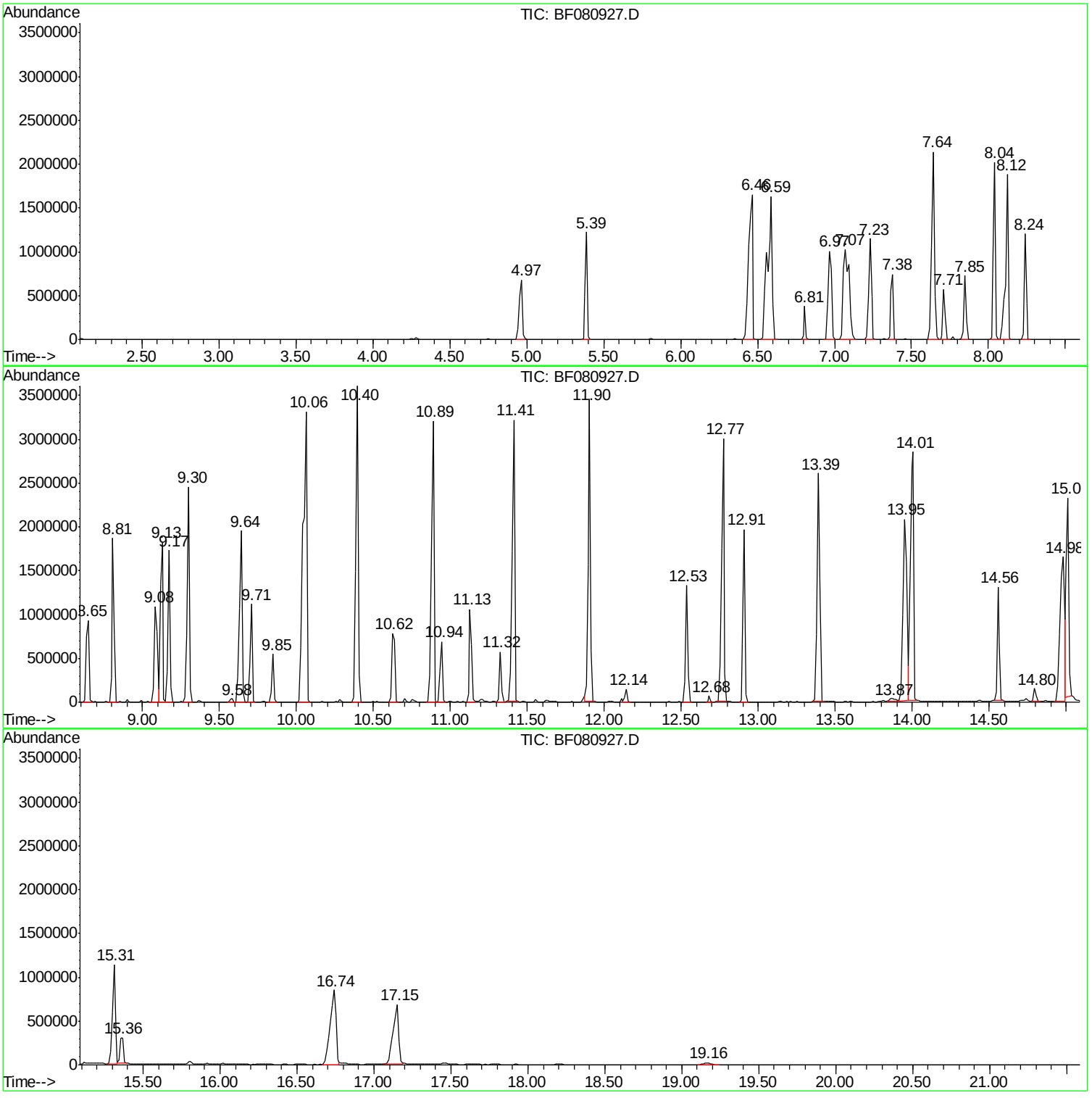
Sum of corrected areas: 96095254

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080715\
Data File : BF080927.D
Acq On : 7 Aug 2015 15:20
Operator : TP/UM
Sample : G3083-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
8524

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080715\
Data File : BF080927.D
Acq On : 7 Aug 2015 15:20
Operator : TP/UM
Sample : G3083-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 8524

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

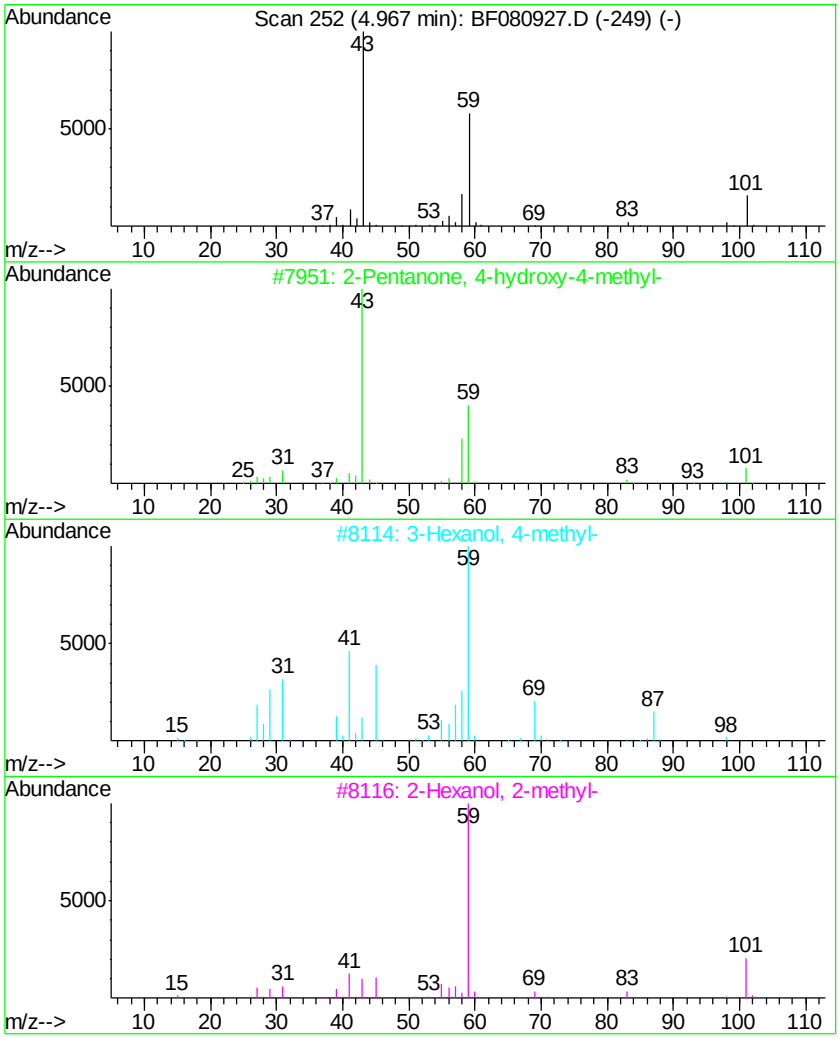
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

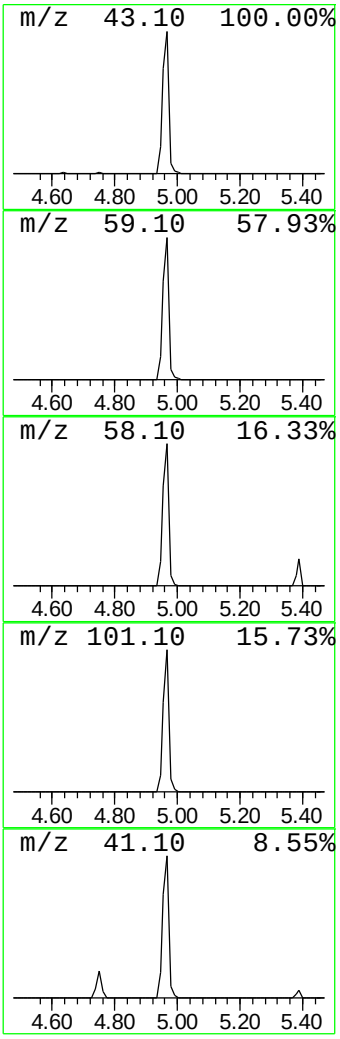
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.97 | 60.82 ng | 920861 | 1,4-Dichlorobenzene-d4 | 6.81 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 3 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 33 |
| 4 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23 |
| 5 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 17 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080715\
Data File : BF080927.D
Acq On : 7 Aug 2015 15:20
Operator : TP/UM
Sample : G3083-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 8524

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

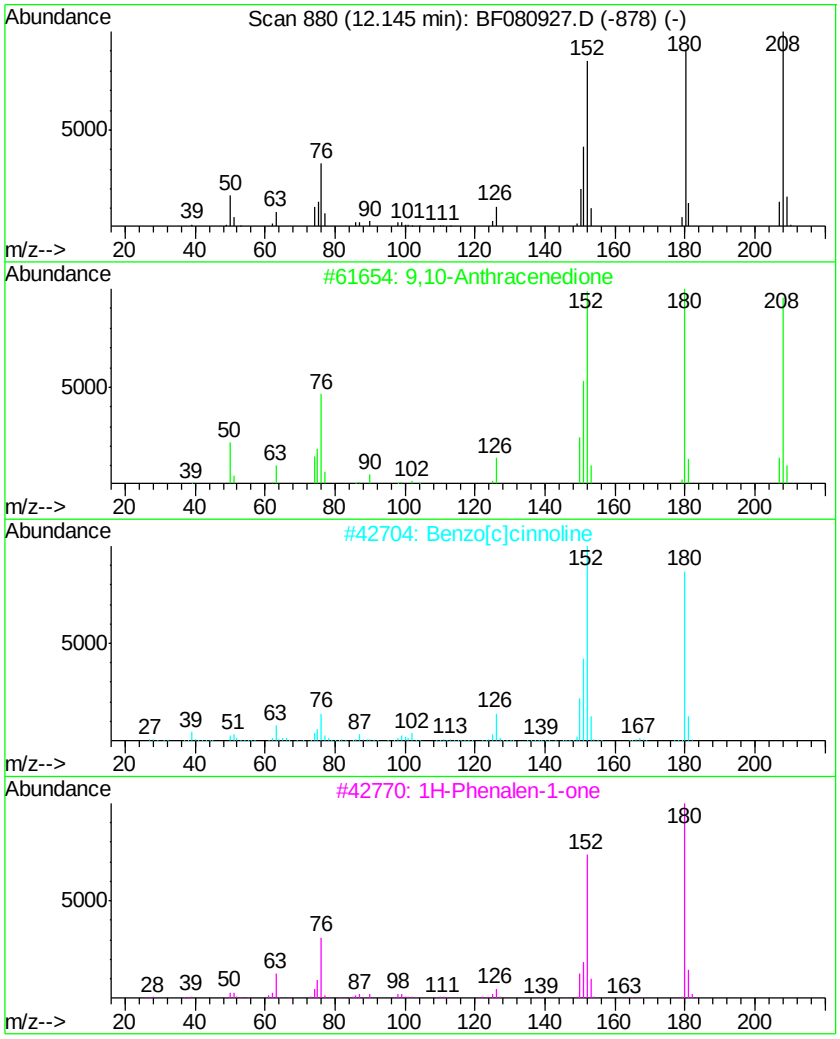
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

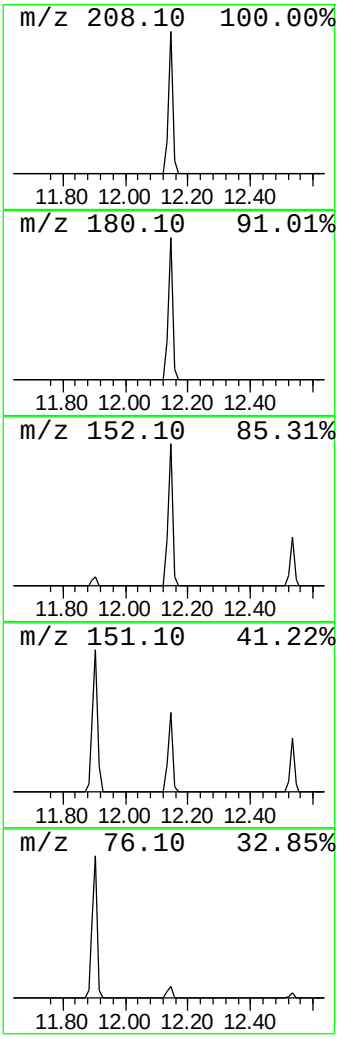
**********

Peak Number 2 9,10-Anthracenedione Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.14 | 5.83 ng | 145346 | Phenanthrene-d10 | 11.32 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9,10-Anthracenedione | 208 | C14H8O2 | 000084-65-1 | 99 |
| 2 | Benzo[c]cinnoline | 180 | C12H8N2 | 000230-17-1 | 86 |
| 3 | 1H-Phenalen-1-one | 180 | C13H8O | 000548-39-0 | 60 |
| 4 | Benzo[h]cinnoline | 180 | C12H8N2 | 000230-31-9 | 60 |
| 5 | 1,4-Anthracenedione | 208 | C14H8O2 | 000635-12-1 | 58 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080715\
Data File : BF080927.D
Acq On : 7 Aug 2015 15:20
Operator : TP/UM
Sample : G3083-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 8524

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

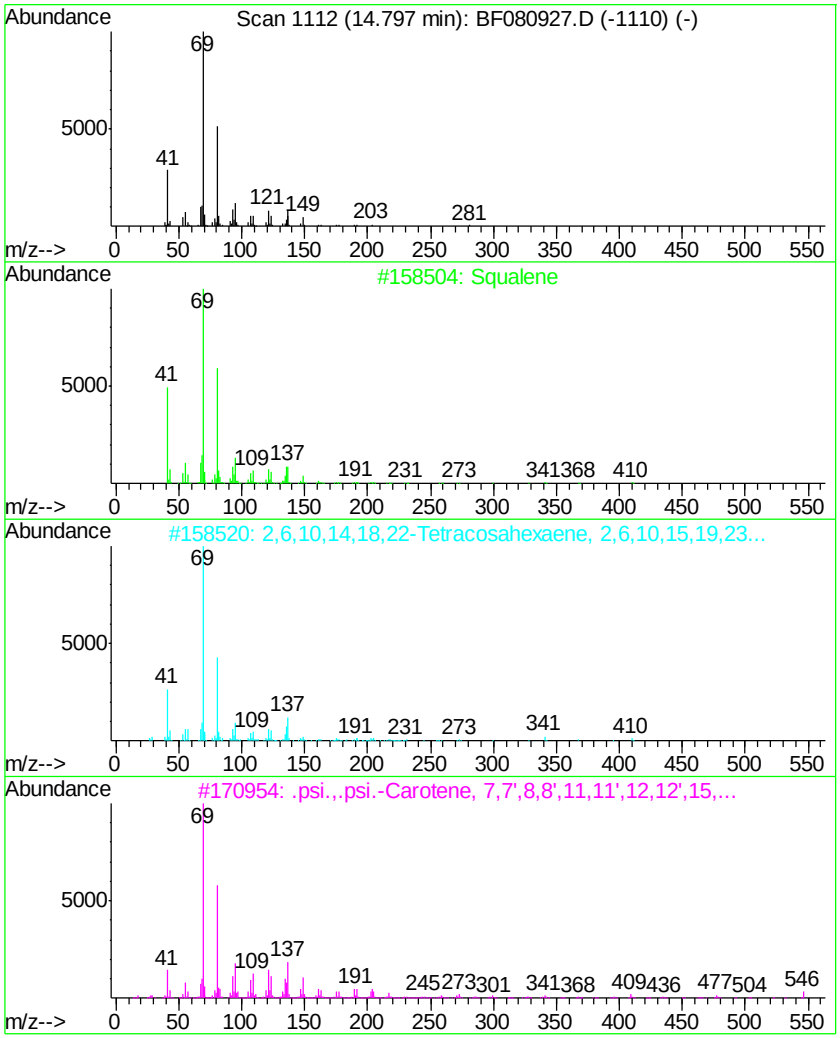
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

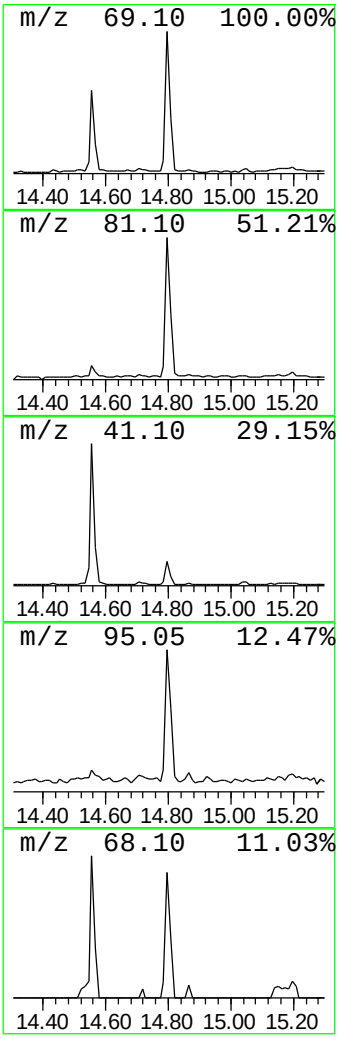
**********

Peak Number 3 Squalene Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.80 | 7.32 ng | 155431 | Perylene-d12 | 15.37 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Squalene | 410 | C30H50 | 007683-64-9 | 91 |
| 2 | 2,6,10,14,18,22-Tetracosahexaene... | 410 | C30H50 | 000111-02-4 | 91 |
| 3 | .psi.,.psi.-Carotene, 7,7',8,8',... | 547 | C40H66 | 000502-62-5 | 83 |
| 4 | 2,6,10-Dodecatrien-1-ol, 3,7,11-... | 222 | C15H26O | 000106-28-5 | 78 |
| 5 | Farnesol isomer a | 222 | C15H26O | 1000108-92-4 | 72 |



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Sample : G3083-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 8524

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

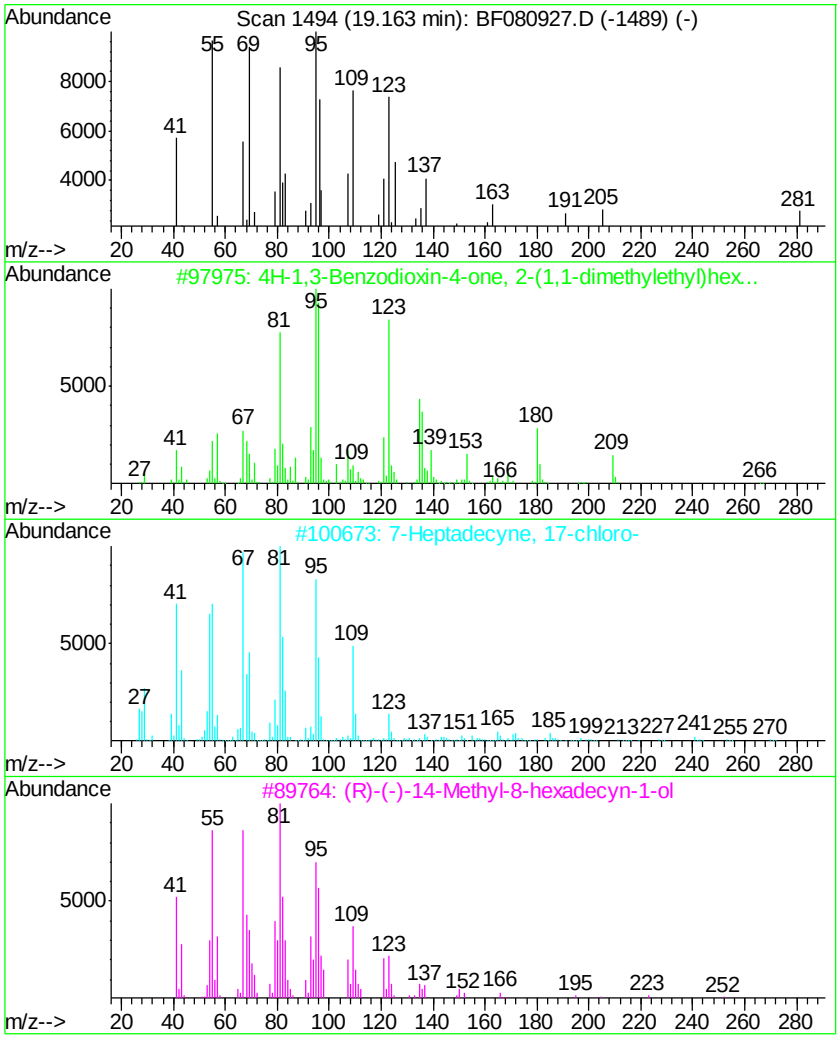
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

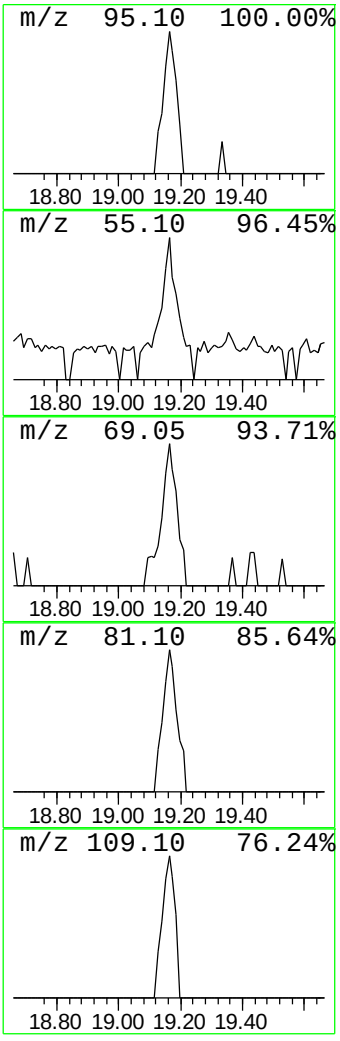
**********

Peak Number 4 unknown19.16 Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.16 | 2.80 ng | 59508 | Perylene-d12 | 15.37 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4H-1,3-Benzodioxin-4-one, 2-(1,1... | 266 | C16H26O3 | 124899-18-9 | 38 |
| 2 | 7-Heptadecyne, 17-chloro- | 270 | C17H31Cl | 056554-75-7 | 38 |
| 3 | (R)-(-)-14-Methyl-8-hexadecyn-1-ol | 252 | C17H32O | 064566-18-3 | 35 |
| 4 | 5-Eicosyne | 278 | C20H38 | 074685-31-7 | 35 |
| 5 | 3-Cyclopentylpropionic acid, but... | 194 | C12H18O2 | 1000292-46-4 | 35 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080715\
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Acq On : 7 Aug 2015 15:20
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Sample : G3083-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 8524

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 4.97 | 60.8 | ng | 920861 | 1 | 6.81 | 302796 | 20.0 |
| 9,10-Anthracenedione | 12.14 | 5.8 | ng | 145346 | 4 | 11.32 | 498573 | 20.0 |
| Squalene | 14.80 | 7.3 | ng | 155431 | 6 | 15.37 | 424424 | 20.0 |
| unknown19.16 | 19.16 | 2.8 | ng | 59508 | 6 | 15.37 | 424424 | 20.0 |