LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088924.D
Acq On : 12 Jul 2016 15:25
Operator : UM/SJ
Sample : H3889-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-6

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-BF063016.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 | 1.678 | 6 | 8 | 16 | rVB | 36693 | 89234 | 4.36% | 0.357% |
| 2 | 1.792 | 16 | 18 | 56 | rVB | 823444 | 1426015 | 69.66% | 5.704% |
| 3 | 4.856 | 283 | 286 | 291 | rBB | 79012 | 119942 | 5.86% | 0.480% |
| 4 | 5.290 | 321 | 324 | 327 | rBV | 1479548 | 1476030 | 72.11% | 5.904% |
| 5 | 6.353 | 413 | 417 | 419 | rVB | 1375098 | 1819779 | 88.90% | 7.279% |
| 6 | 6.467 | 425 | 427 | 430 | rBV | 1349222 | 1590702 | 77.71% | 6.362% |
| 7 | 6.639 | 440 | 442 | 444 | rBV | 30148 | 25530 | 1.25% | 0.102% |
| 8 | 6.707 | 445 | 448 | 449 | rBV | 362791 | 430622 | 21.04% | 1.722% |
| 9 | 6.856 | 459 | 461 | 464 | rVB | 1127205 | 1218714 | 59.54% | 4.875% |
| 10 | 7.267 | 494 | 497 | 500 | rBV | 915168 | 961076 | 46.95% | 3.844% |
| 11 | 7.382 | 503 | 507 | 510 | rBV2 | 29306 | 55094 | 2.69% | 0.220% |
| 12 | 7.736 | 536 | 538 | 540 | rBV2 | 21628 | 27531 | 1.34% | 0.110% |
| 13 | 7.987 | 558 | 560 | 562 | rBV | 710879 | 594624 | 29.05% | 2.378% |
| 14 | 8.342 | 589 | 591 | 594 | rBV | 21593 | 20518 | 1.00% | 0.082% |
| 15 | 8.753 | 625 | 627 | 630 | rBV | 30225 | 32562 | 1.59% | 0.130% |
| 16 | 9.073 | 652 | 655 | 657 | rBV | 1875048 | 2046993 | 100.00% | 8.187% |
| 17 | 9.462 | 687 | 689 | 691 | rBV | 315596 | 245954 | 12.02% | 0.984% |
| 18 | 9.656 | 704 | 706 | 708 | rBV | 46182 | 39606 | 1.93% | 0.158% |
| 19 | 9.736 | 711 | 713 | 715 | rBV | 657362 | 592714 | 28.96% | 2.371% |
| 20 | 9.770 | 715 | 716 | 718 | rVB | 104651 | 72551 | 3.54% | 0.290% |
| 21 | 9.885 | 724 | 726 | 728 | rBV | 48505 | 42351 | 2.07% | 0.169% |
| 22 | 9.942 | 728 | 731 | 733 | rVV | 35592 | 31965 | 1.56% | 0.128% |
| 23 | 10.285 | 759 | 761 | 763 | rVB | 45566 | 50525 | 2.47% | 0.202% |
| 24 | 10.342 | 763 | 766 | 770 | rBV2 | 9942 | 26807 | 1.31% | 0.107% |
| 25 | 10.525 | 779 | 782 | 784 | rVB | 1037360 | 1003249 | 49.01% | 4.013% |
| 26 | 10.650 | 791 | 793 | 798 | rBV | 35800 | 53544 | 2.62% | 0.214% |
| 27 | 11.016 | 824 | 825 | 827 | rVB | 30602 | 24444 | 1.19% | 0.098% |
| 28 | 11.085 | 827 | 831 | 834 | rBV2 | 87016 | 197883 | 9.67% | 0.791% |
| 29 | 11.211 | 840 | 842 | 843 | rBV | 523175 | 482672 | 23.58% | 1.931% |
| 30 | 11.291 | 846 | 849 | 851 | rVB | 102652 | 128930 | 6.30% | 0.516% |
| 31 | 11.439 | 860 | 862 | 864 | rVV2 | 75879 | 77885 | 3.80% | 0.312% |
| 32 | 11.531 | 867 | 870 | 873 | rVB2 | 15019 | 34223 | 1.67% | 0.137% |
| 33 | 11.713 | 884 | 886 | 887 | rBV | 41707 | 34035 | 1.66% | 0.136% |
| 34 | 11.759 | 887 | 890 | 891 | rVV2 | 70462 | 98627 | 4.82% | 0.394% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088924.D
Acq On : 12 Jul 2016 15:25
Operator : UM/SJ
Sample : H3889-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-6

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-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 11.782 | 891 | 892 | 894 | rVB | 20654 | 21716 | 1.06% | 0.087% |
| 36 | 11.828 | 894 | 896 | 900 | rBV | 90545 | 123841 | 6.05% | 0.495% |
| 37 | 11.896 | 900 | 902 | 904 | rBV | 21102 | 27014 | 1.32% | 0.108% |
| 38 | 12.011 | 910 | 912 | 915 | rVB2 | 30979 | 57748 | 2.82% | 0.231% |
| 39 | 12.262 | 932 | 934 | 936 | rBV2 | 18918 | 25847 | 1.26% | 0.103% |
| 40 | 12.342 | 940 | 941 | 945 | rVV3 | 26361 | 35426 | 1.73% | 0.142% |
| 41 | 12.422 | 945 | 948 | 950 | rVB | 629186 | 617904 | 30.19% | 2.471% |
| 42 | 12.548 | 957 | 959 | 964 | rBV3 | 16450 | 45324 | 2.21% | 0.181% |
| 43 | 12.639 | 964 | 967 | 969 | rBV2 | 394811 | 553144 | 27.02% | 2.212% |
| 44 | 12.685 | 969 | 971 | 975 | rVB3 | 27105 | 49134 | 2.40% | 0.197% |
| 45 | 12.765 | 976 | 978 | 979 | rBV | 32686 | 30807 | 1.50% | 0.123% |
| 46 | 12.799 | 979 | 981 | 983 | rVB | 1398576 | 1282518 | 62.65% | 5.130% |
| 47 | 12.868 | 983 | 987 | 988 | rBV | 28141 | 42790 | 2.09% | 0.171% |
| 48 | 12.971 | 991 | 996 | 998 | rVB2 | 70341 | 98329 | 4.80% | 0.393% |
| 49 | 13.039 | 998 | 1002 | 1003 | rBV | 65248 | 81128 | 3.96% | 0.324% |
| 50 | 13.074 | 1003 | 1005 | 1006 | rVV | 54263 | 52556 | 2.57% | 0.210% |
| 51 | 13.096 | 1006 | 1007 | 1009 | rVB | 37267 | 36305 | 1.77% | 0.145% |
| 52 | 13.256 | 1019 | 1021 | 1026 | rVB3 | 9381 | 22786 | 1.11% | 0.091% |
| 53 | 13.336 | 1026 | 1028 | 1030 | rBV | 36251 | 59449 | 2.90% | 0.238% |
| 54 | 13.474 | 1037 | 1040 | 1043 | rBV | 55722 | 70689 | 3.45% | 0.283% |
| 55 | 13.588 | 1047 | 1050 | 1051 | rBV2 | 54113 | 76301 | 3.73% | 0.305% |
| 56 | 13.611 | 1051 | 1052 | 1053 | rVV | 36050 | 39842 | 1.95% | 0.159% |
| 57 | 13.702 | 1057 | 1060 | 1063 | rVV2 | 106047 | 174728 | 8.54% | 0.699% |
| 58 | 13.839 | 1067 | 1072 | 1076 | rBV2 | 608980 | 1136402 | 55.52% | 4.545% |
| 59 | 13.942 | 1077 | 1081 | 1083 | rBV | 61756 | 92991 | 4.54% | 0.372% |
| 60 | 14.022 | 1086 | 1088 | 1089 | rVV | 42648 | 47830 | 2.34% | 0.191% |
| 61 | 14.057 | 1089 | 1091 | 1093 | rVB2 | 27474 | 45218 | 2.21% | 0.181% |
| 62 | 14.159 | 1098 | 1100 | 1101 | rBV2 | 22957 | 21172 | 1.03% | 0.085% |
| 63 | 14.217 | 1103 | 1105 | 1107 | rVV | 33217 | 48464 | 2.37% | 0.194% |
| 64 | 14.251 | 1107 | 1108 | 1110 | rVB2 | 24296 | 29013 | 1.42% | 0.116% |
| 65 | 14.331 | 1113 | 1115 | 1120 | rVV3 | 175196 | 256355 | 12.52% | 1.025% |
| 66 | 14.422 | 1121 | 1123 | 1125 | rVB2 | 31764 | 39527 | 1.93% | 0.158% |
| 67 | 14.514 | 1130 | 1131 | 1133 | rBV2 | 24125 | 36401 | 1.78% | 0.146% |
| 68 | 14.685 | 1144 | 1146 | 1150 | rVB2 | 58221 | 82179 | 4.01% | 0.329% |
| 69 | 14.834 | 1156 | 1159 | 1163 | rBV | 288455 | 534556 | 26.11% | 2.138% |
| 70 | 14.925 | 1164 | 1167 | 1172 | rVV2 | 346549 | 499224 | 24.39% | 1.997% |
| 71 | 15.028 | 1172 | 1176 | 1177 | rVV3 | 33748 | 69454 | 3.39% | 0.278% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088924.D
Acq On : 12 Jul 2016 15:25
Operator : UM/SJ
Sample : H3889-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-6

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-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 72 | 15.097 | 1180 | 1182 | 1185 | rVB | 162339 | 205523 | 10.04% | 0.822% |
| 73 | 15.154 | 1185 | 1187 | 1189 | rBV | 221493 | 235973 | 11.53% | 0.944% |
| 74 | 15.211 | 1189 | 1192 | 1198 | rBV2 | 372217 | 514661 | 25.14% | 2.058% |
| 75 | 15.440 | 1210 | 1212 | 1214 | rBV2 | 23437 | 29982 | 1.46% | 0.120% |
| 76 | 15.645 | 1227 | 1230 | 1232 | rBV | 188972 | 277430 | 13.55% | 1.110% |
| 77 | 15.691 | 1232 | 1234 | 1238 | rVB2 | 102621 | 168682 | 8.24% | 0.675% |
| 78 | 15.874 | 1248 | 1250 | 1253 | rVB2 | 24629 | 37255 | 1.82% | 0.149% |
| 79 | 15.988 | 1258 | 1260 | 1264 | rVB4 | 20264 | 47114 | 2.30% | 0.188% |
| 80 | 16.091 | 1266 | 1269 | 1272 | rBV3 | 16762 | 46931 | 2.29% | 0.188% |
| 81 | 16.491 | 1301 | 1304 | 1311 | rBV2 | 95195 | 207017 | 10.11% | 0.828% |
| 82 | 16.605 | 1311 | 1314 | 1316 | rVV | 55259 | 104763 | 5.12% | 0.419% |
| 83 | 16.651 | 1316 | 1318 | 1325 | rVB5 | 34356 | 131744 | 6.44% | 0.527% |
| 84 | 16.880 | 1334 | 1338 | 1344 | rVB | 66069 | 140083 | 6.84% | 0.560% |
| 85 | 17.017 | 1345 | 1350 | 1353 | rBV3 | 111985 | 278714 | 13.62% | 1.115% |
| 86 | 17.085 | 1353 | 1356 | 1357 | rBV | 19056 | 31447 | 1.54% | 0.126% |
| 87 | 17.200 | 1363 | 1366 | 1371 | rVB2 | 44650 | 112093 | 5.48% | 0.448% |
| 88 | 17.291 | 1372 | 1374 | 1377 | rBV4 | 13365 | 31370 | 1.53% | 0.125% |
| 89 | 17.394 | 1380 | 1383 | 1390 | rVB4 | 33326 | 109262 | 5.34% | 0.437% |
| 90 | 17.908 | 1424 | 1428 | 1435 | rVB4 | 45131 | 144301 | 7.05% | 0.577% |
| 91 | 18.663 | 1489 | 1494 | 1502 | rBV3 | 36494 | 130728 | 6.39% | 0.523% |
| 92 | 18.811 | 1502 | 1507 | 1517 | rVB4 | 78387 | 279691 | 13.66% | 1.119% |

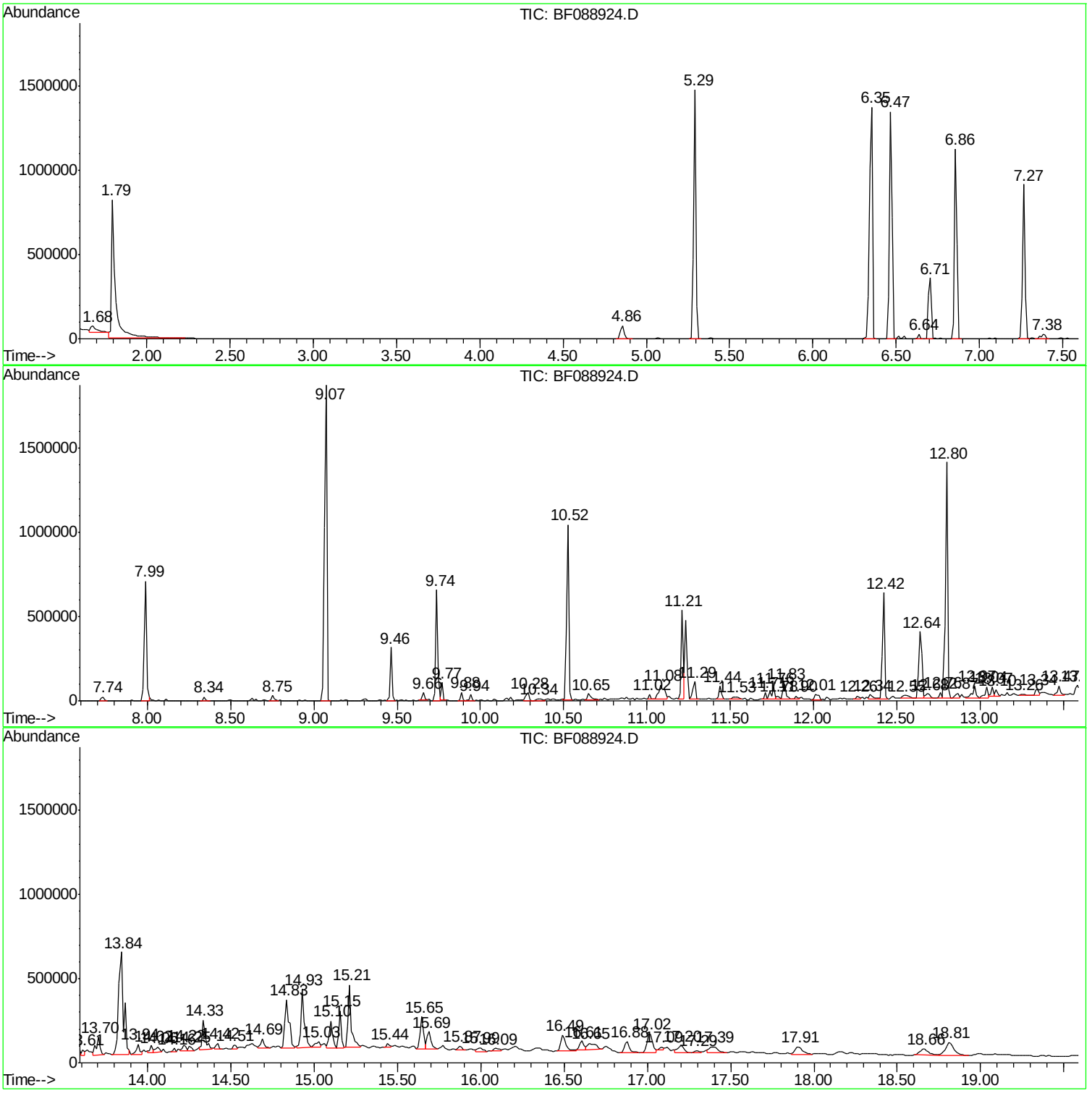
Sum of corrected areas: 25001807

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088924.D
Acq On : 12 Jul 2016 15:25
Operator : UM/SJ
Sample : H3889-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
SS-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088924.D
Acq On : 12 Jul 2016 15:25
Operator : UM/SJ
Sample : H3889-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

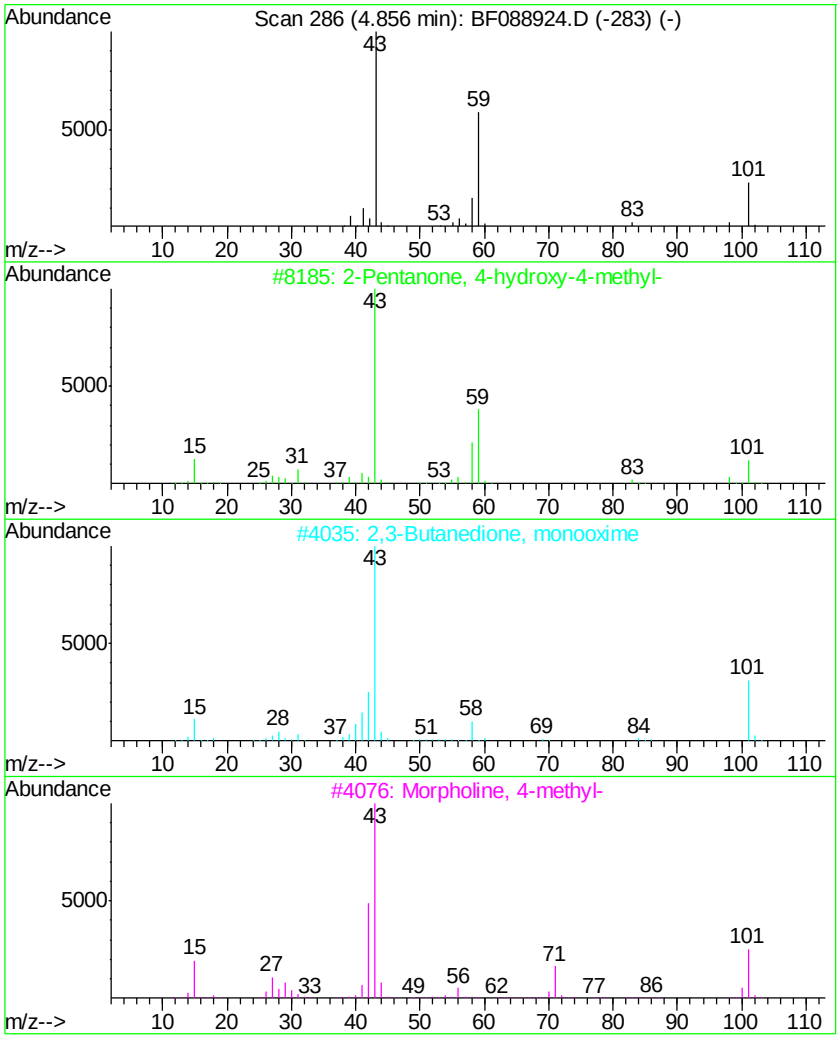
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

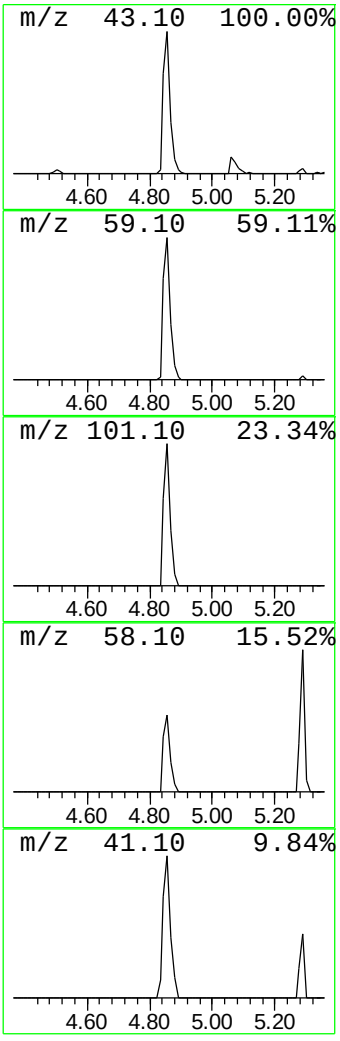
**********

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.86 | 5.57 ng | 119942 | 1,4-Dichlorobenzene-d4 | 6.71 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 25 |
| 3 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 4 | (+-)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 9 |
| 5 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088924.D
Acq On : 12 Jul 2016 15:25
Operator : UM/SJ
Sample : H3889-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

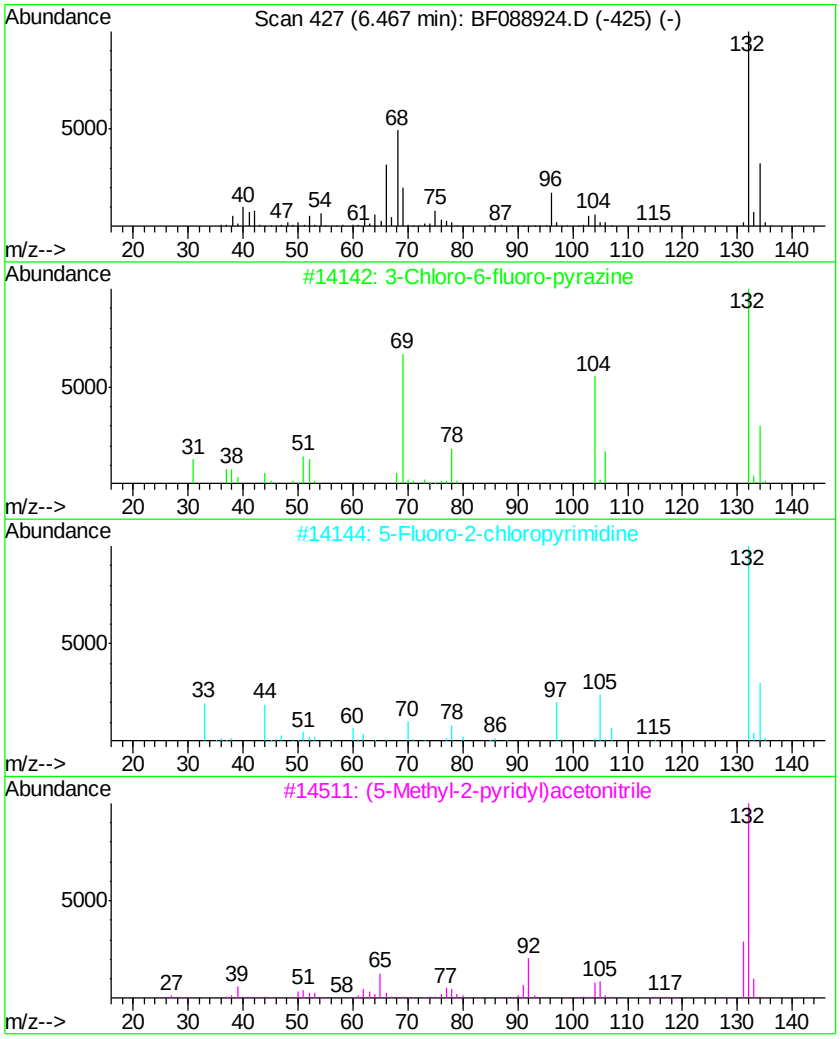
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

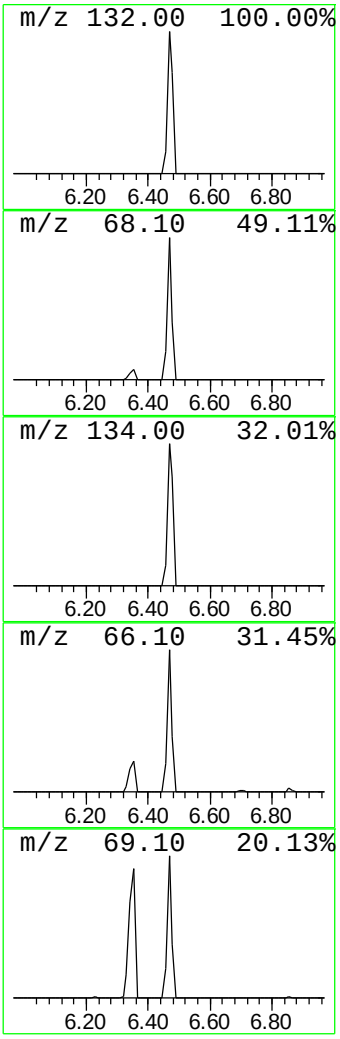
**********

Peak Number 4 unknown6.47 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.47 | 73.88 ng | 1590700 | 1,4-Dichlorobenzene-d4 | 6.71 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 12 |
| 3 | (5-Methyl-2-pyridyl)acetonitrile | 132 | C8H8N2 | 1000241-93-9 | 10 |
| 4 | Cyclopropanamine, 1-phenyl- | 133 | C9H11N | 1000351-26-2 | 10 |
| 5 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088924.D
Acq On : 12 Jul 2016 15:25
Operator : UM/SJ
Sample : H3889-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

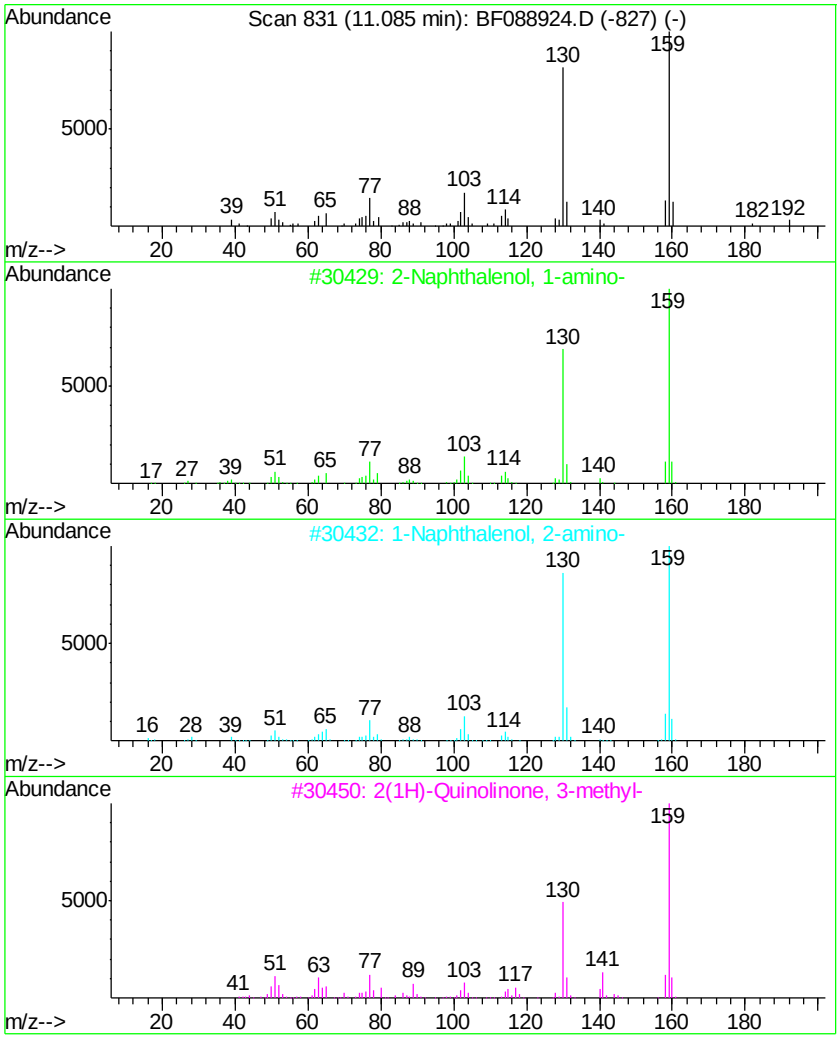
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

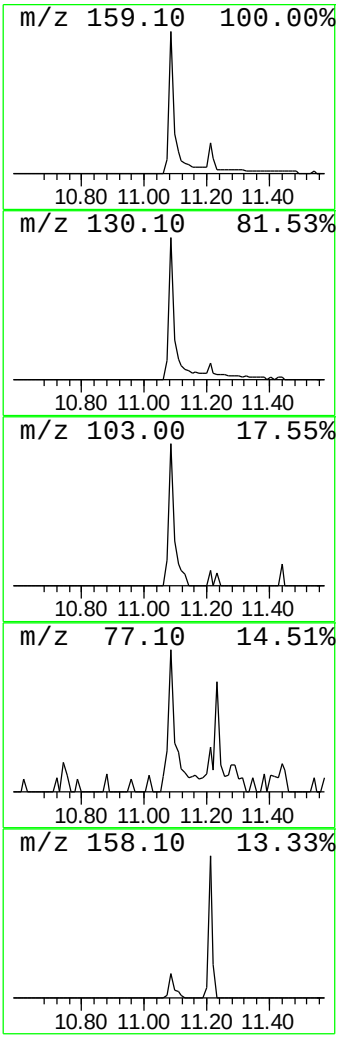
**********

Peak Number 6 2-Naphthalenol, 1-amino- Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.08 | 8.20 ng | 197883 | Phenanthrene-d10 | 11.21 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Naphthalenol, 1-amino- | 159 | C10H9NO | 002834-92-6 | 97 |
| 2 | 1-Naphthalenol, 2-amino- | 159 | C10H9NO | 000606-41-7 | 94 |
| 3 | 2(1H)-Quinolinone, 3-methyl- | 159 | C10H9NO | 002721-59-7 | 91 |
| 4 | 8-Quinolinol, 7-methyl- | 159 | C10H9NO | 005541-68-4 | 87 |
| 5 | 5-Amino-1-naphthol | 159 | C10H9NO | 000083-55-6 | 80 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088924.D
Acq On : 12 Jul 2016 15:25
Operator : UM/SJ
Sample : H3889-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

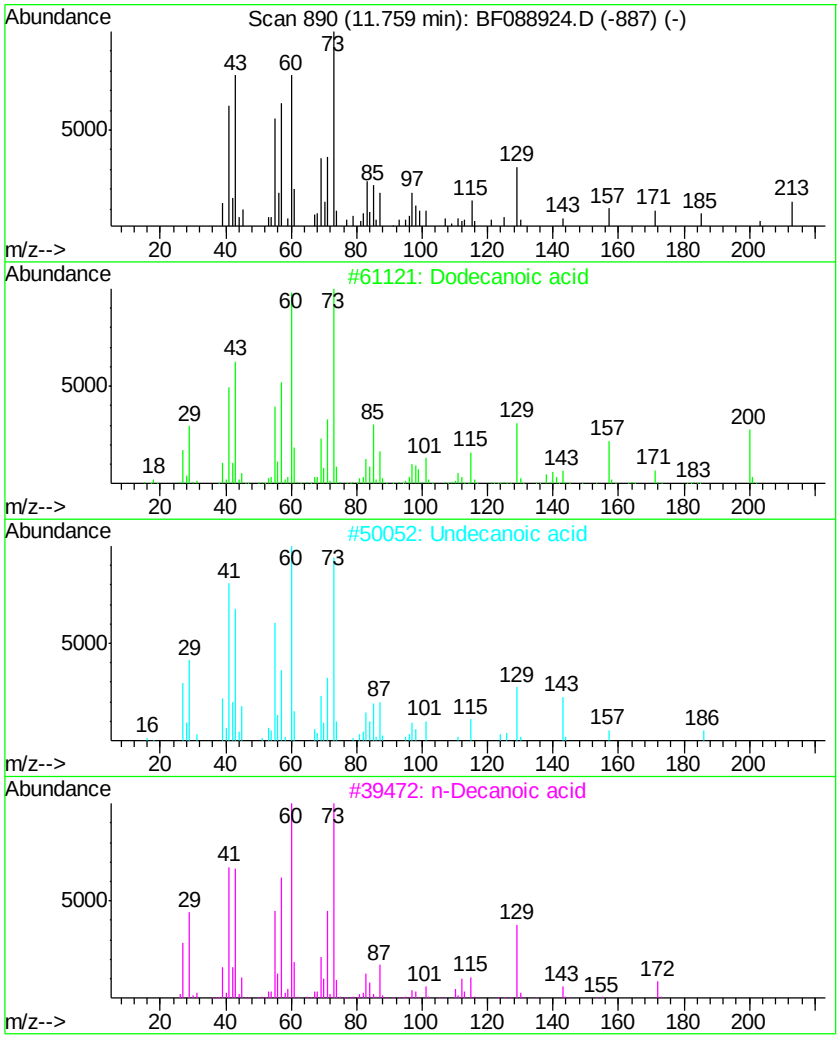
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

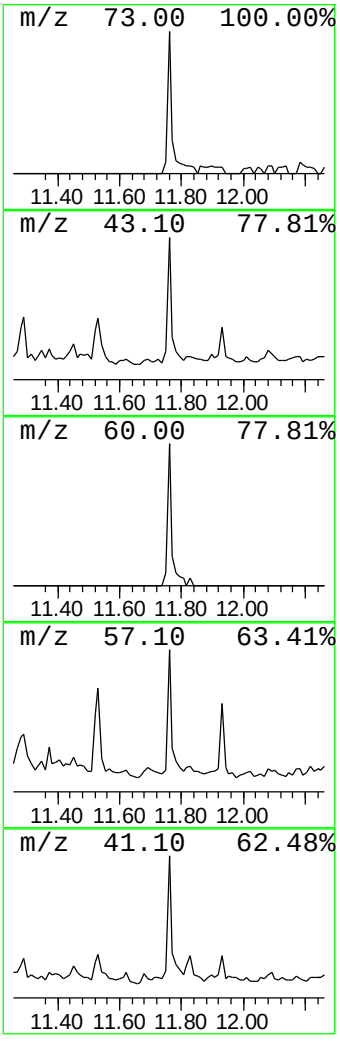
**********

Peak Number 7 Dodecanoic acid Concentration Rank 20

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.76 | 4.09 ng | 98627 | Phenanthrene-d10 | 11.21 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 64 |
| 2 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 59 |
| 3 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 53 |
| 4 | d-Glucohexodialdose | 178 | C6H10O6 | 1000149-19-1 | 50 |
| 5 | n-Capric acid isopropyl ester | 214 | C13H26O2 | 002311-59-3 | 50 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088924.D
Acq On : 12 Jul 2016 15:25
Operator : UM/SJ
Sample : H3889-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

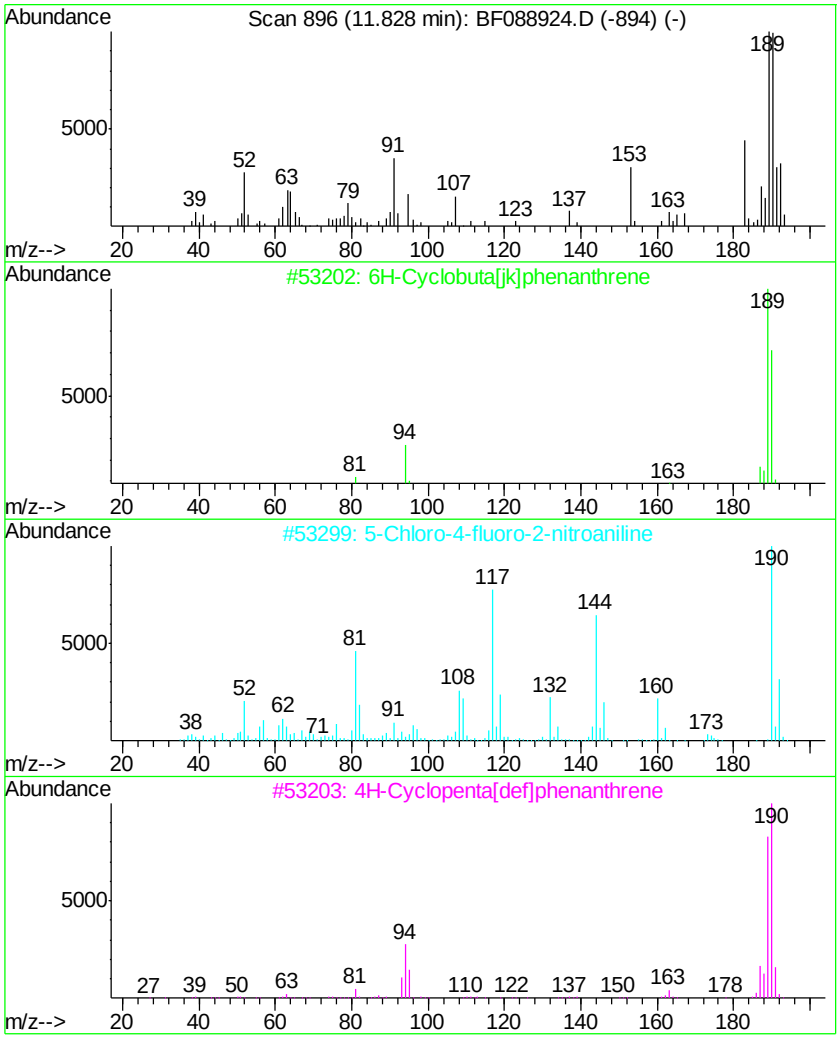
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

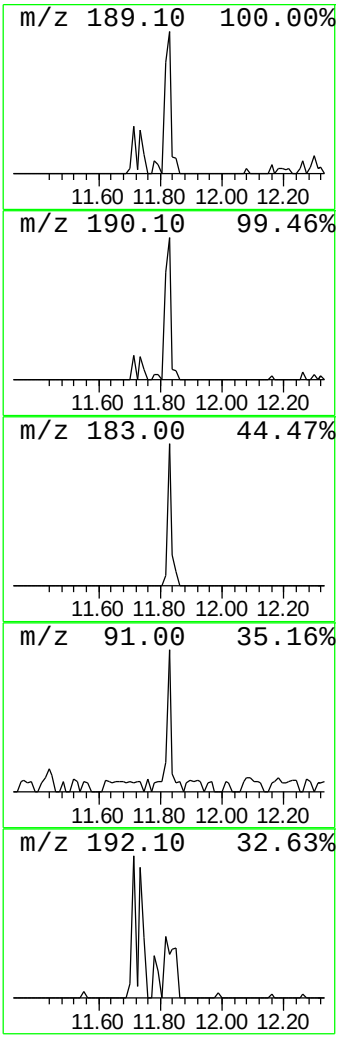
**********

Peak Number 8 6H-Cyclobuta[jk]phenanthrene Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.83 | 5.13 ng | 123841 | Phenanthrene-d10 | 11.21 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 6H-Cyclobuta[jk]phenanthrene | 190 | C15H10 | 083469-43-6 | 50 |
| 2 | 5-Chloro-4-fluoro-2-nitroaniline | 190 | C6H4ClFN2O2 | 104222-34-6 | 43 |
| 3 | 4H-Cyclopenta[def]phenanthrene | 190 | C15H10 | 000203-64-5 | 43 |
| 4 | 3-(Trifluoromethoxy)benzaldehyde | 190 | C8H5F3O2 | 052771-21-8 | 38 |
| 5 | (5,6-Dihydro-2H-[1,4]oxazin-3-yl... | 190 | C11H14N2O | 1000295-04-4 | 30 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088924.D
Acq On : 12 Jul 2016 15:25
Operator : UM/SJ
Sample : H3889-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

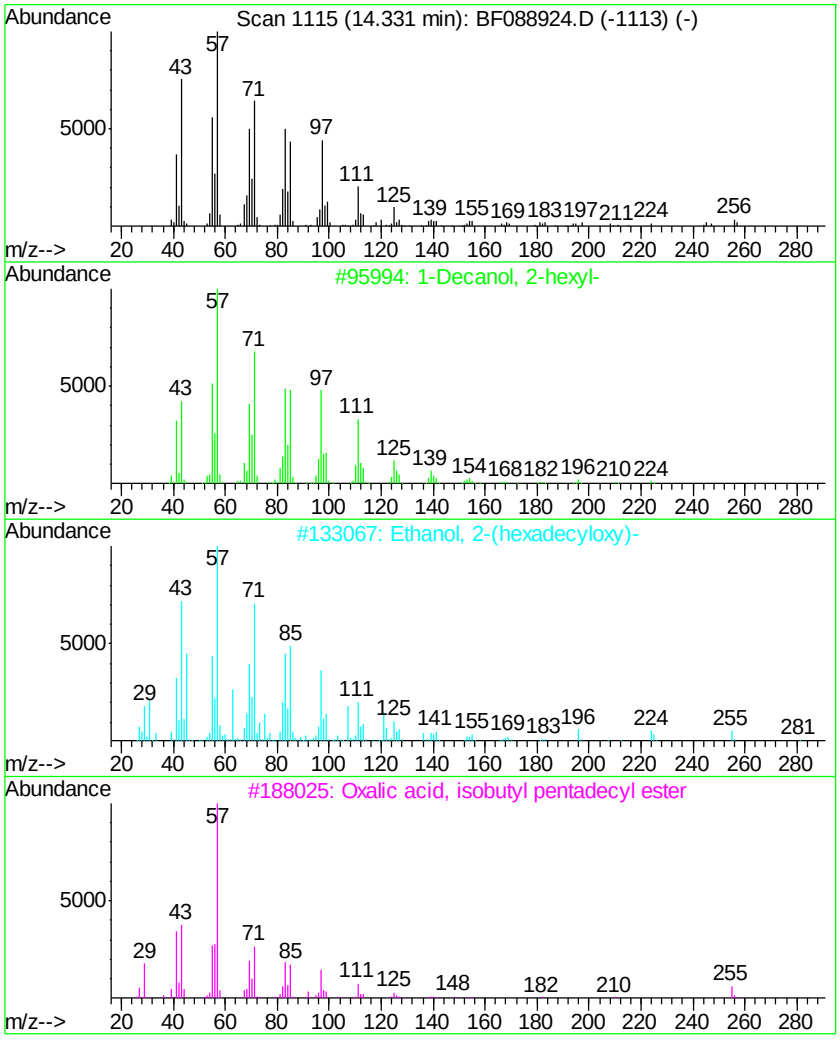
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

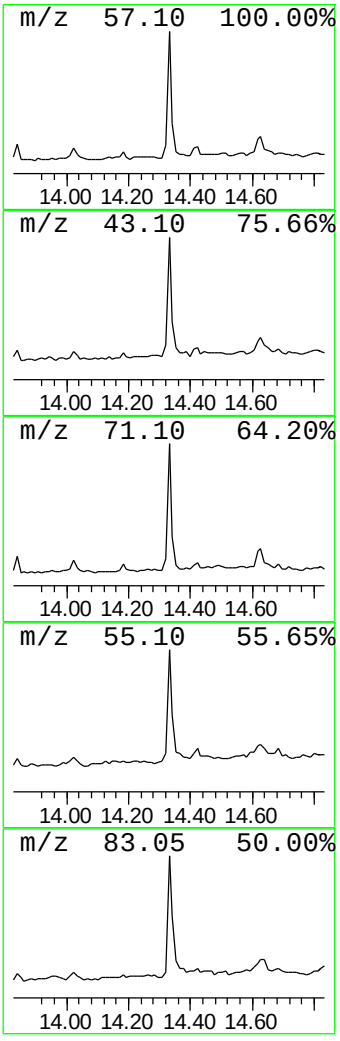
**********

Peak Number 9 1-Decanol, 2-hexyl- Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.33 | 4.51 ng | 256355 | Chrysene-d12 | 13.84 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Decanol, 2-hexyl- | 242 | C16H34O | 002425-77-6 | 91 |
| 2 | Ethanol, 2-(hexadecyloxy)- | 286 | C18H38O2 | 002136-71-2 | 91 |
| 3 | Oxalic acid, isobutyl pentadecyl... | 356 | C21H40O4 | 1000309-38-0 | 91 |
| 4 | Heptafluorobutyric acid, n-octad... | 466 | C22H37F7O2 | 000400-57-7 | 81 |
| 5 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 76 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088924.D
Acq On : 12 Jul 2016 15:25
Operator : UM/SJ
Sample : H3889-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

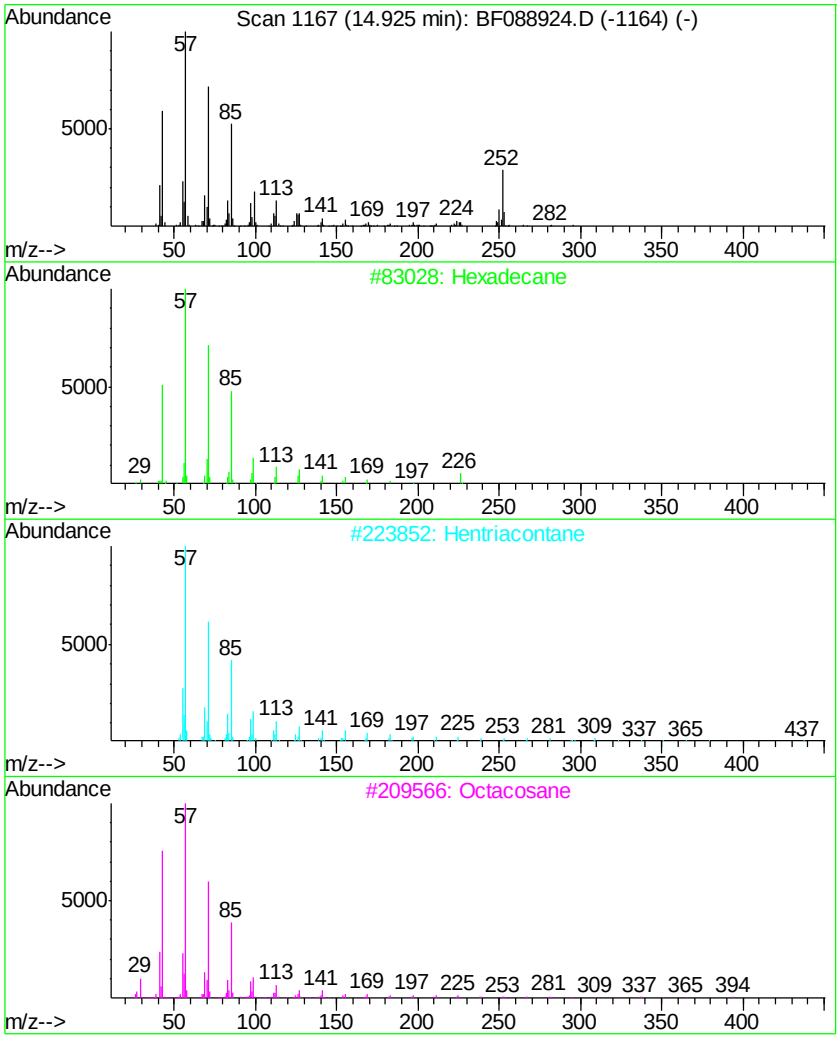
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

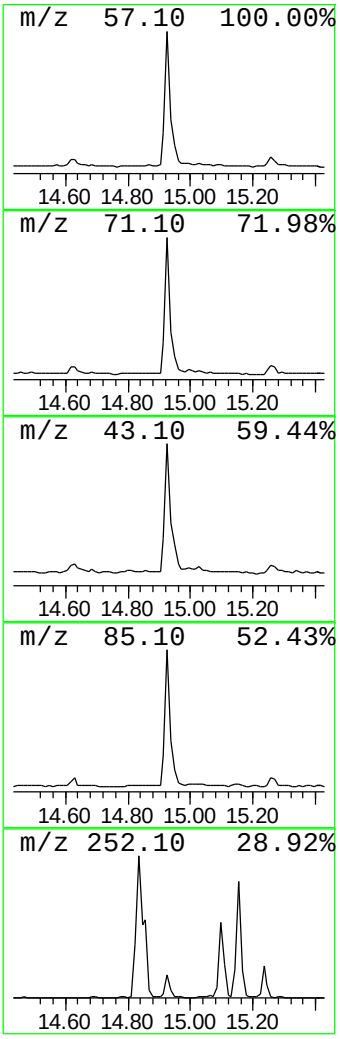
**********

Peak Number 10 Hexadecane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.93 | 19.40 ng | 499224 | Perylene-d12 | 15.21 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane | 226 | C16H34 | 000544-76-3 | 95 |
| 2 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 81 |
| 3 | Octacosane | 394 | C28H58 | 000630-02-4 | 81 |
| 4 | Heneicosane | 296 | C21H44 | 000629-94-7 | 81 |
| 5 | Pentacosane | 352 | C25H52 | 000629-99-2 | 74 |



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Data File : BF088924.D
Acq On : 12 Jul 2016 15:25
Operator : UM/SJ
Sample : H3889-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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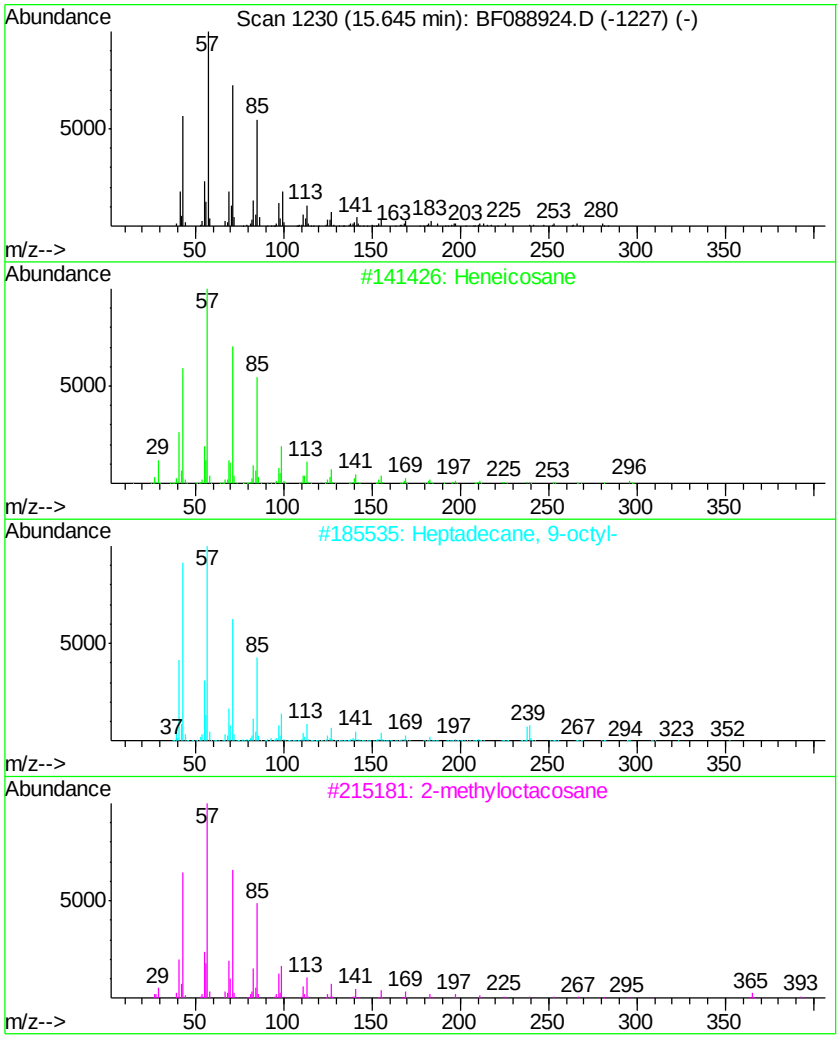
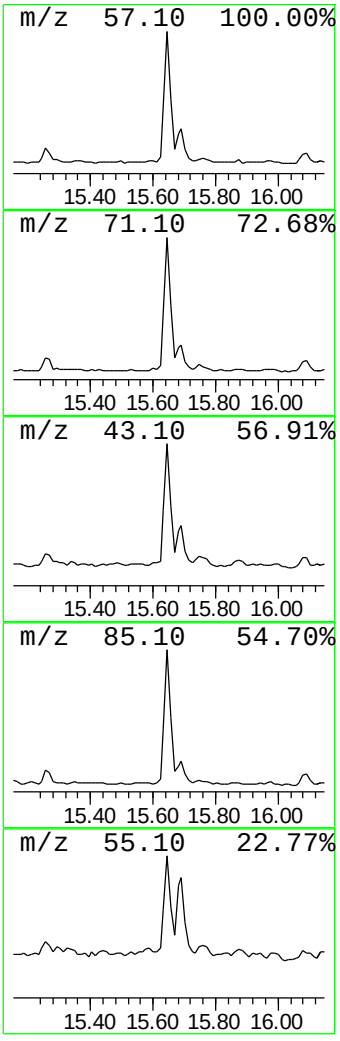
Peak Number 12 Heneicosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.65 | 10.78 ng | 277430 | Perylene-d12 | 15.21 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 2 | Heptadecane, 9-octyl- | 352 | C25H52 | 007225-64-1 | 91 |
| 3 | 2-methyloctacosane | 408 | C29H60 | 1000376-72-8 | 91 |
| 4 | Hexacosane | 366 | C26H54 | 000630-01-3 | 90 |
| 5 | Heptadecane | 240 | C17H36 | 000629-78-7 | 87 |



# Library Search Compound Report

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Data File : BF088924.D
Acq On : 12 Jul 2016 15:25
Operator : UM/SJ
Sample : H3889-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

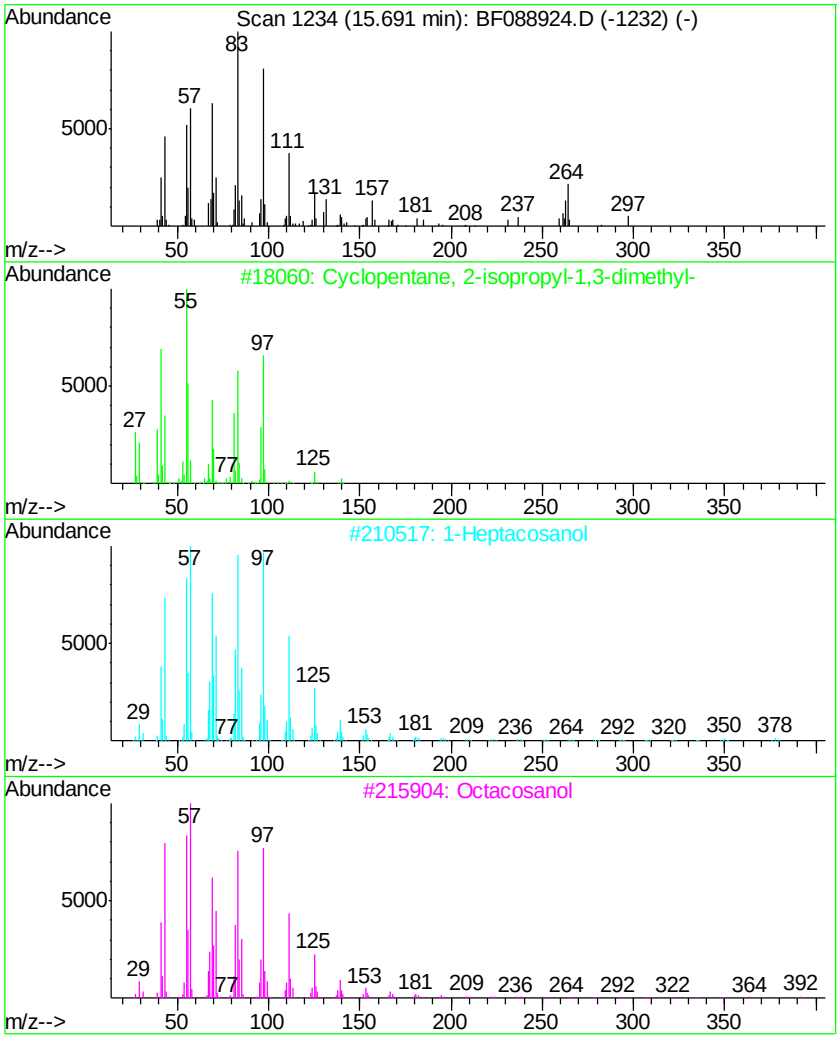
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

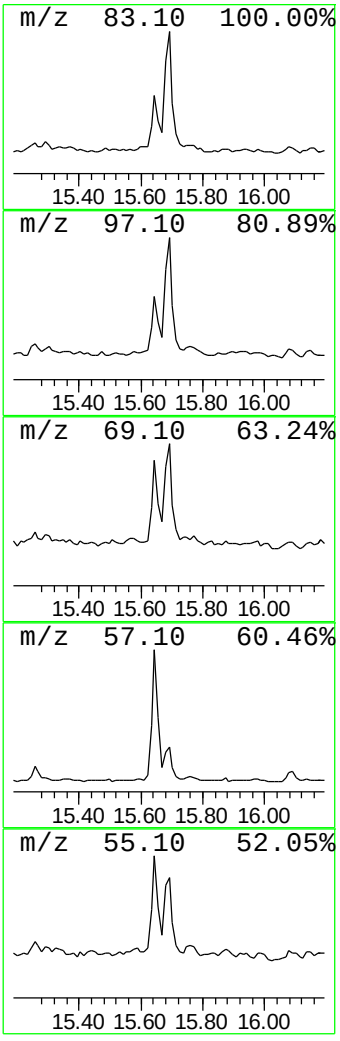
**********

Peak Number 13 Cyclopentane, 2-isopropyl-1... Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.69 | 6.56 ng | 168682 | Perylene-d12 | 15.21 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclopentane, 2-isopropyl-1,3-di... | 140 | C10H20 | 032281-85-9 | 52 |
| 2 | 1-Heptacosanol | 396 | C27H56O | 002004-39-9 | 42 |
| 3 | Octacosanol | 410 | C28H58O | 000557-61-9 | 42 |
| 4 | Cycloheptane, methyl- | 112 | C8H16 | 004126-78-7 | 38 |
| 5 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 38 |



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Data File : BF088924.D
Acq On : 12 Jul 2016 15:25
Operator : UM/SJ
Sample : H3889-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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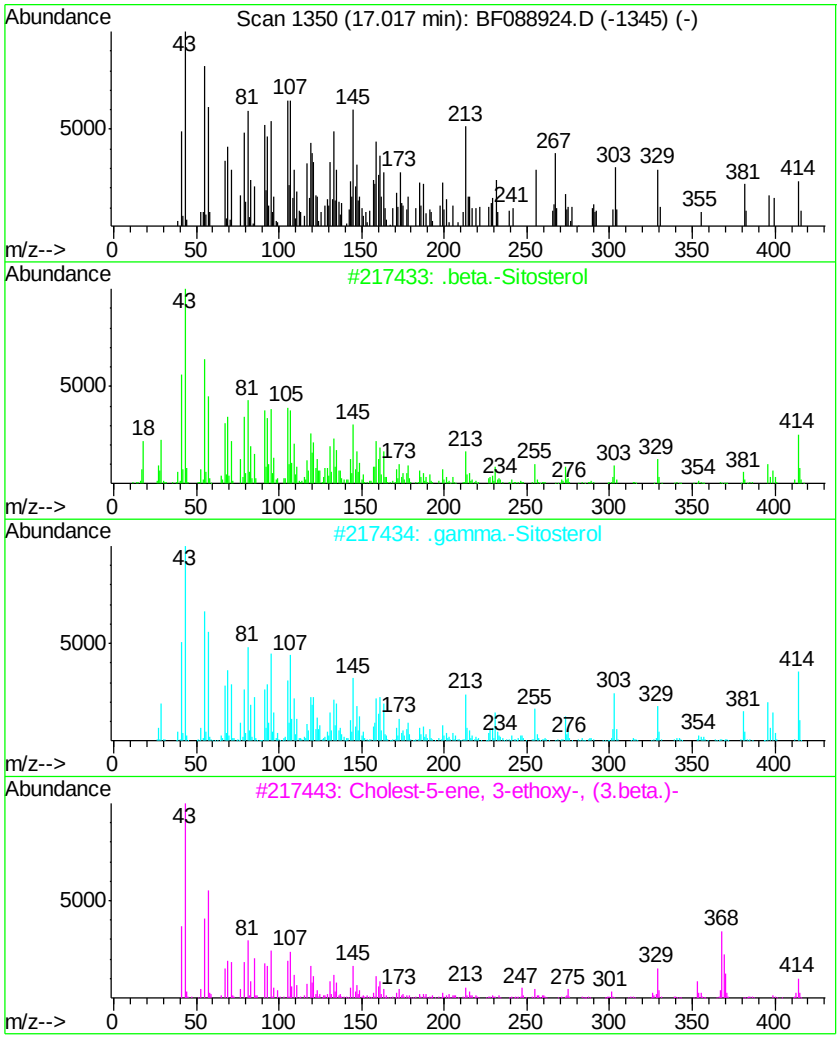
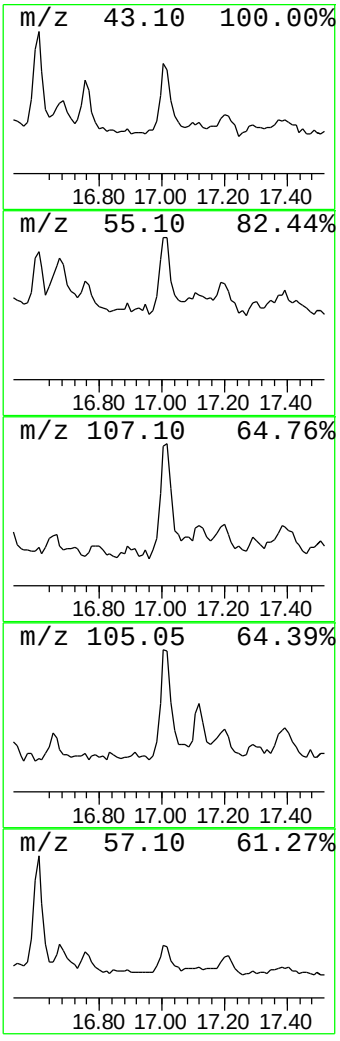
Peak Number 15 .beta.-Sitosterol Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.02 | 10.83 ng | 278714 | Perylene-d12 | 15.21 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | .beta.-Sitosterol | 414 | C29H50O | 000083-46-5 | 99 |
| 2 | .gamma.-Sitosterol | 414 | C29H50O | 000083-47-6 | 95 |
| 3 | Cholest-5-ene, 3-ethoxy-, (3.bet... | 414 | C29H50O | 000986-19-6 | 70 |
| 4 | Pregn-5-en-3-ol, 21-bromo-20-met... | 394 | C22H35BrO | 055103-80-5 | 22 |
| 5 | .beta.-Sitosterol acetate | 456 | C31H52O2 | 000915-05-9 | 16 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088924.D
Acq On : 12 Jul 2016 15:25
Operator : UM/SJ
Sample : H3889-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

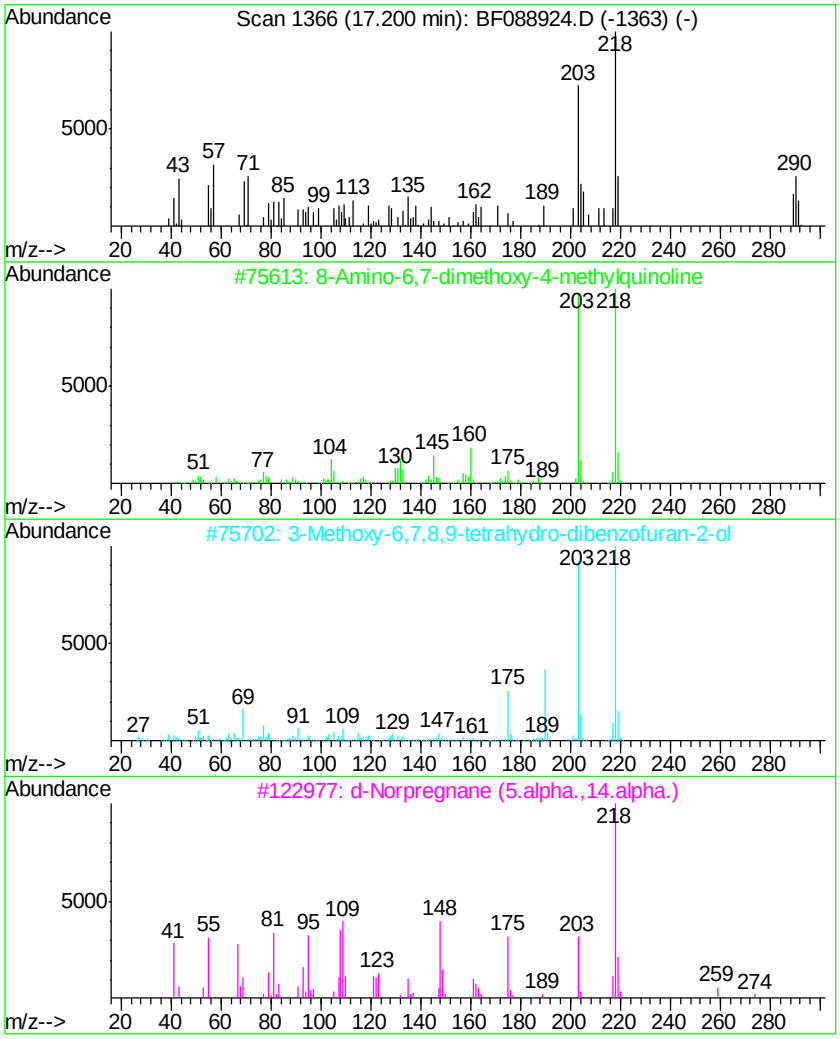
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

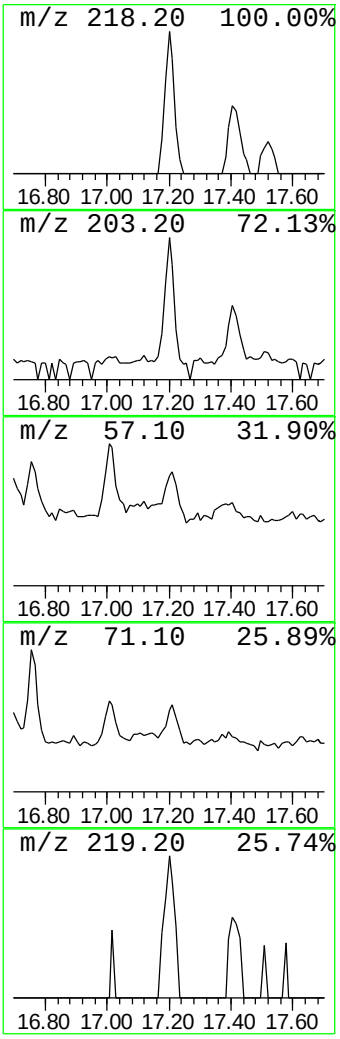
**********

Peak Number 16 unknown17.20 Concentration Rank 17

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.20 | 4.36 ng | 112093 | Perylene-d12 | 15.21 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 8-Amino-6,7-dimethoxy-4-methylqu... | 218 | C12H14N2O2 | 1000213-07-2 | 47 |
| 2 | 3-Methoxy-6,7,8,9-tetrahydro-dib... | 218 | C13H14O3 | 1000186-57-9 | 47 |
| 3 | d-Norpregnane (5.alpha.,14.alpha.) | 274 | C20H34 | 1000281-13-7 | 43 |
| 4 | 4H-Benz[de]anthracene, 5,6-dihydro- | 218 | C17H14 | 004389-09-7 | 43 |
| 5 | Indolizine, 1-acetyl-2-methyl-6-... | 218 | C11H10N2O3 | 1000071-33-1 | 43 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088924.D
Acq On : 12 Jul 2016 15:25
Operator : UM/SJ
Sample : H3889-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

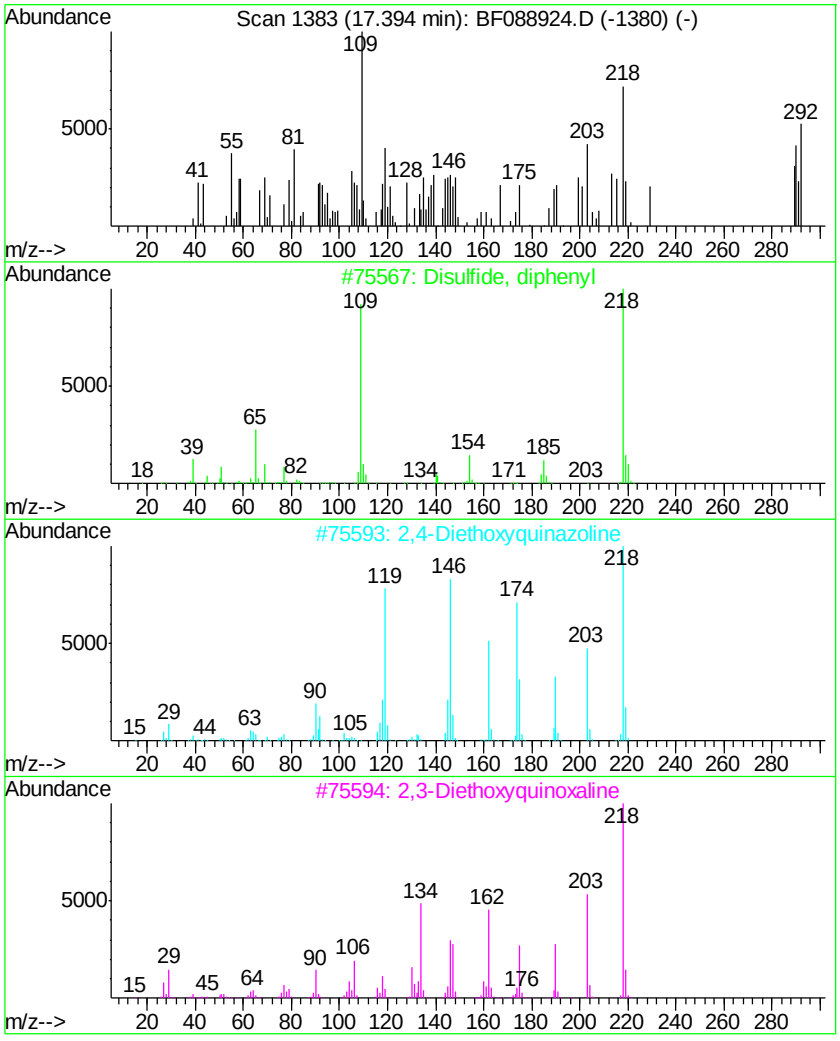
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

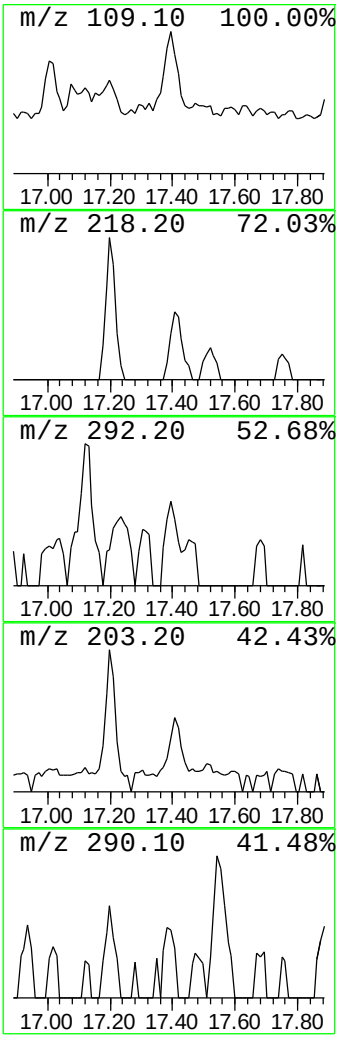
**********

Peak Number 17 unknown17.39 Concentration Rank 18

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.39 | 4.25 ng | 109262 | Perylene-d12 | 15.21 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Disulfide, diphenyl | 218 | C12H10S2 | 000882-33-7 | 22 |
| 2 | 2,4-Diethoxyquinazoline | 218 | C12H14N2O2 | 000611-65-4 | 18 |
| 3 | 2,3-Diethoxyquinoxaline | 218 | C12H14N2O2 | 057050-66-5 | 15 |
| 4 | 2,5,8- Trimethyl-1-nonen-3-yn-5-ol | 180 | C12H20O | 208173-17-5 | 14 |
| 5 | 4-(2-Propyn-1-yloxy)phenol | 148 | C9H8O2 | 034596-27-5 | 11 |



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Data File : BF088924.D
Acq On : 12 Jul 2016 15:25
Operator : UM/SJ
Sample : H3889-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

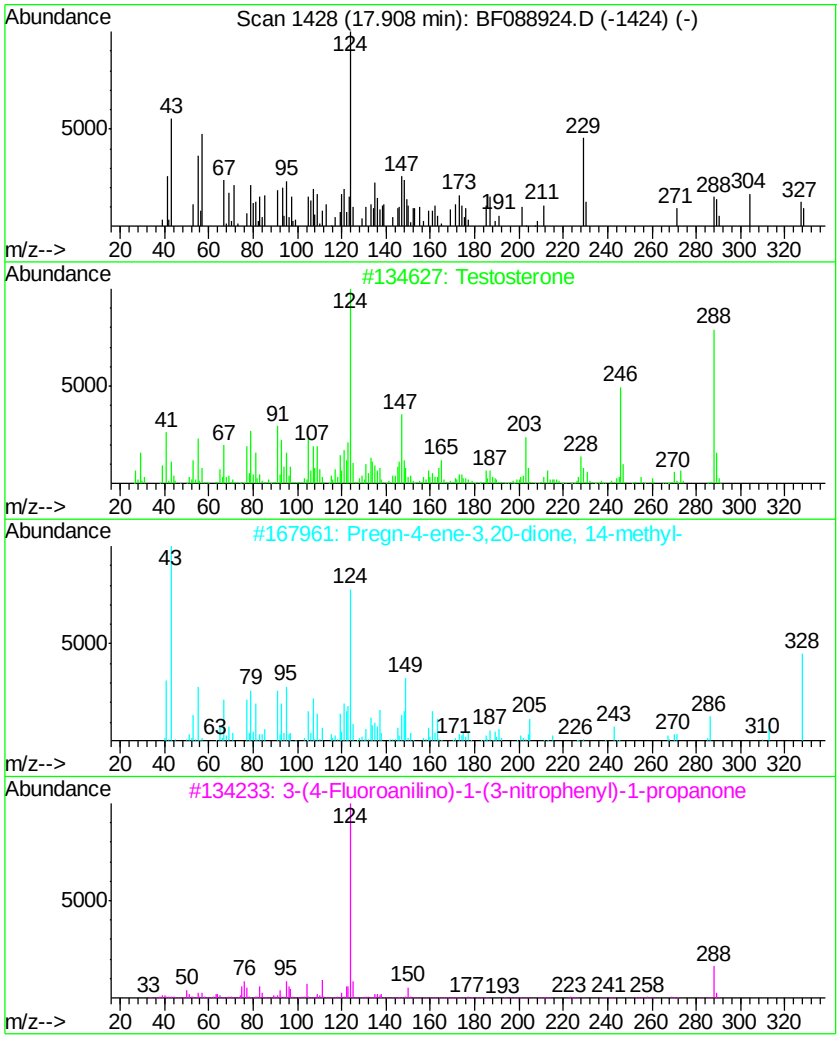
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

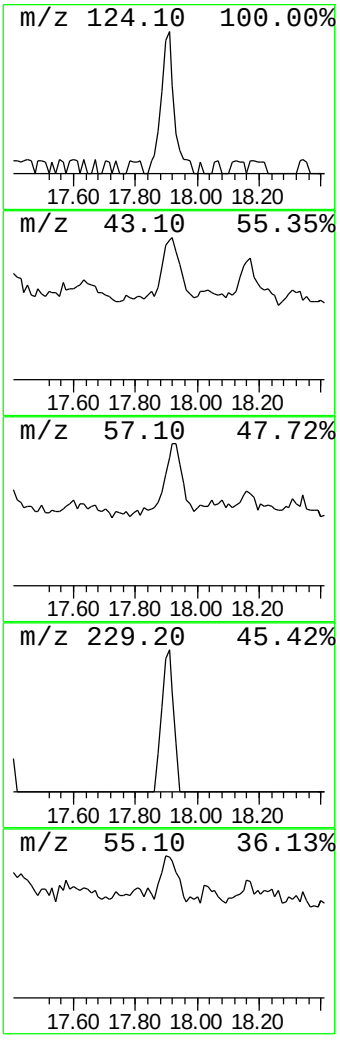
**********

Peak Number 18 unknown17.91 Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.91 | 5.61 ng | 144301 | Perylene-d12 | 15.21 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Testosterone | 288 | C19H28O2 | 000058-22-0 | 46 |
| 2 | Pregn-4-ene-3,20-dione, 14-methyl- | 328 | C22H32O2 | 055162-96-4 | 38 |
| 3 | 3-(4-Fluoroanilino)-1-(3-nitroph... | 288 | C15H13FN2O3 | 350039-84-8 | 30 |
| 4 | N-Methyl-N-(2,2,6,6-tetramethyl-... | 342 | C18H26N6O | 1000295-16-2 | 27 |
| 5 | 3-(3-Fluoroanilino)-1-(3-nitroph... | 288 | C15H13FN2O3 | 300726-64-1 | 27 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
Data File : BF088924.D
Acq On : 12 Jul 2016 15:25
Operator : UM/SJ
Sample : H3889-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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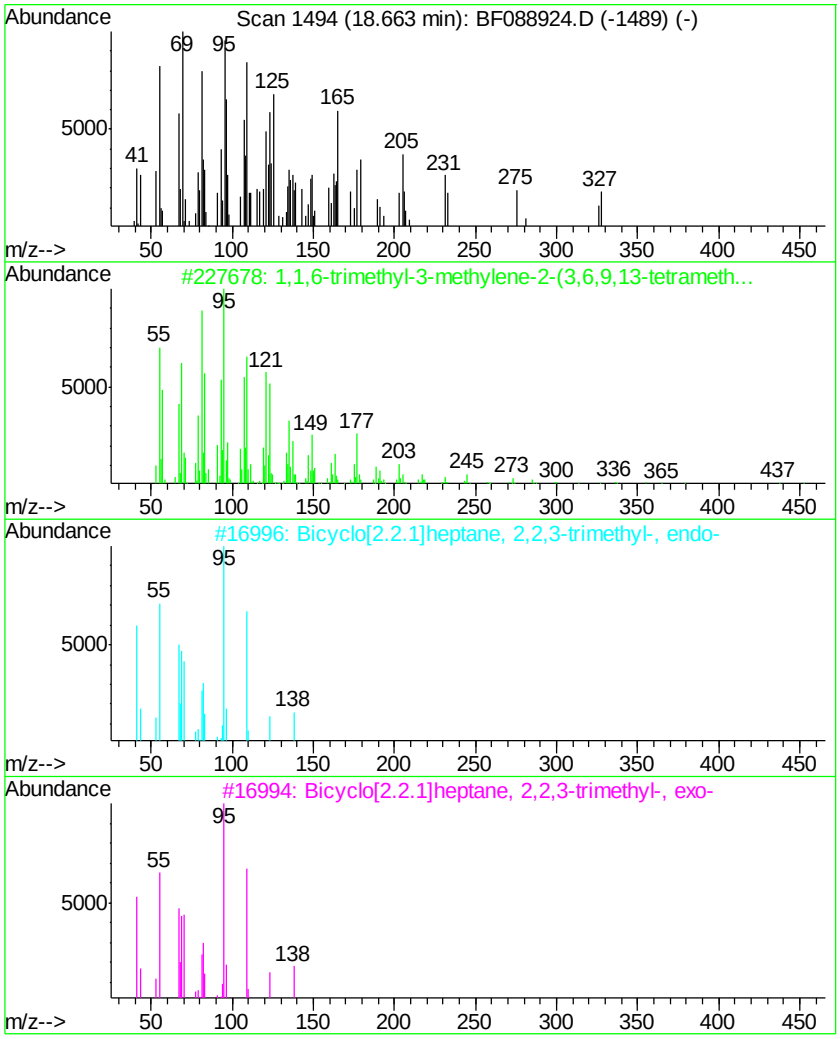
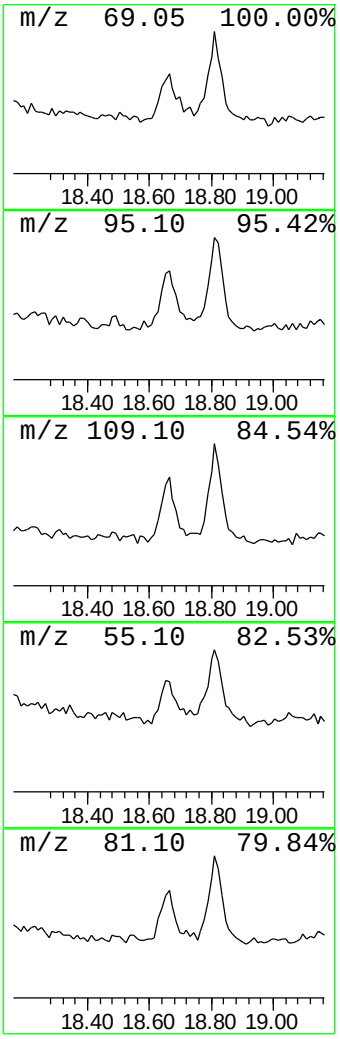
Peak Number 19 unknown18.66 Concentration Rank 15

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.66 | 5.08 ng | 130728 | Perylene-d12 | 15.21 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,1,6-trimethyl-3-methylene-2-(3... | 452 | C33H56 | 1000373-94-5 | 43 |
| 2 | Bicyclo[2.2.1]heptane, 2,2,3-tri... | 138 | C10H18 | 020536-40-7 | 38 |
| 3 | Bicyclo[2.2.1]heptane, 2,2,3-tri... | 138 | C10H18 | 020536-41-8 | 38 |
| 4 | 1-Methylbicyclo[3.2.1]octane | 124 | C9H16 | 119972-41-7 | 38 |
| 5 | 2,4a,8,8-Tetramethyldecahydrocyc... | 206 | C15H26 | 074022-04-1 | 38 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071216\
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Operator : UM/SJ
Sample : H3889-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

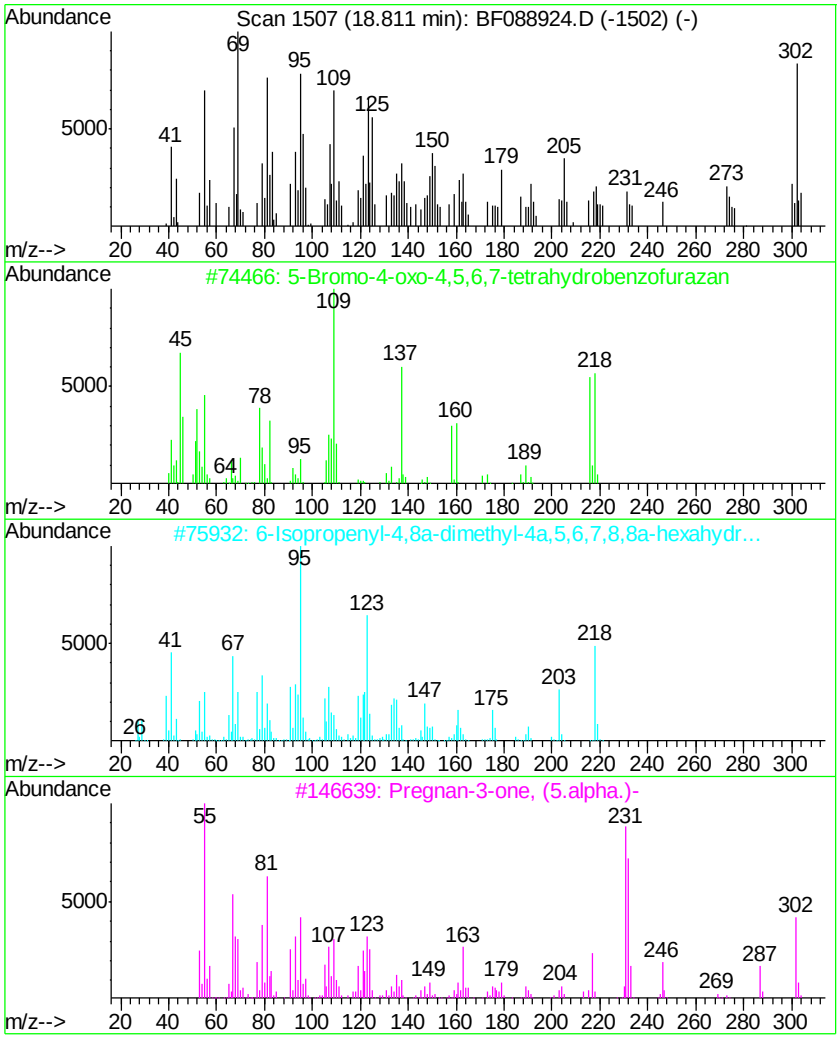
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

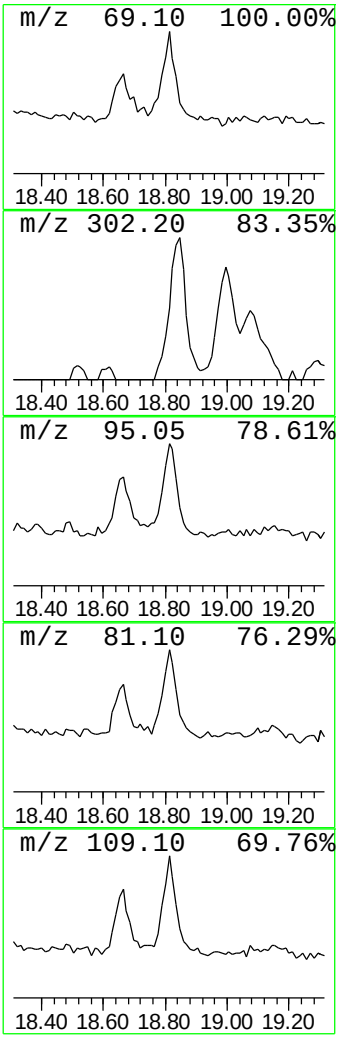
**********

Peak Number 20 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.81 | 10.87 ng | 279691 | Perylene-d12 | 15.21 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Bromo-4-oxo-4,5,6,7-tetrahydro... | 216 | C6H5BrN2O2 | 300574-36-1 | 59 |
| 2 | 6-Isopropenyl-4,8a-dimethyl-4a,5... | 218 | C15H22O | 086917-79-5 | 43 |
| 3 | Pregnan-3-one, (5.alpha.)- | 302 | C21H34O | 014778-11-1 | 43 |
| 4 | 2(1H)-Naphthalenone, 5-[2-(3-fur... | 302 | C20H30O2 | 059742-40-4 | 38 |
| 5 | Cyclohexene, 1-pentyl-4-(4-propy... | 276 | C20H36 | 108067-20-5 | 38 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071216\
Data File : BF088924.D
Acq On : 12 Jul 2016 15:25
Operator : UM/SJ
Sample : H3889-06
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SS-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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 |
| 2-Pentanone, 4-hy... | 4.86 | 5.6 | ng | 119942 | 1 | 6.71 | 430622 | 20.0 |
| unknown6.47 | 6.47 | 73.9 | ng | 1590700 | 1 | 6.71 | 430622 | 20.0 |
| 2-Naphthalenol, 1... | 11.08 | 8.2 | ng | 197883 | 4 | 11.21 | 482672 | 20.0 |
| Dodecanoic acid | 11.76 | 4.1 | ng | 98627 | 4 | 11.21 | 482672 | 20.0 |
| 6H-Cyclobuta[jk]p... | 11.83 | 5.1 | ng | 123841 | 4 | 11.21 | 482672 | 20.0 |
| 1-Decanol, 2-hexyl- | 14.33 | 4.5 | ng | 256355 | 5 | 13.84 | 1136400 | 20.0 |
| Hexadecane | 14.93 | 19.4 | ng | 499224 | 6 | 15.21 | 514661 | 20.0 |
| Heneicosane | 15.65 | 10.8 | ng | 277430 | 6 | 15.21 | 514661 | 20.0 |
| Cyclopentane, 2-i... | 15.69 | 6.6 | ng | 168682 | 6 | 15.21 | 514661 | 20.0 |
| .beta.-Sitosterol | 17.02 | 10.8 | ng | 278714 | 6 | 15.21 | 514661 | 20.0 |
| unknown17.20 | 17.20 | 4.4 | ng | 112093 | 6 | 15.21 | 514661 | 20.0 |
| unknown17.39 | 17.39 | 4.3 | ng | 109262 | 6 | 15.21 | 514661 | 20.0 |
| unknown17.91 | 17.91 | 5.6 | ng | 144301 | 6 | 15.21 | 514661 | 20.0 |
| unknown18.66 | 18.66 | 5.1 | ng | 130728 | 6 | 15.21 | 514661 | 20.0 |
| 5-Bromo-4-oxo-4,5... | 18.81 | 10.9 | ng | 279691 | 6 | 15.21 | 514661 | 20.0 |