LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097074.D
Acq On : 26 Jul 2017 14:40
Operator : SJ/JU
Sample : I4443-05 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** E2-M7-ESW

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-BF072517.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 | 4.710 | 474 | 480 | 483 | rBV | 2390237 | 2941551 | 9.96% | 1.904% |
| 2 | 5.022 | 529 | 533 | 541 | rBV | 620919 | 836834 | 2.83% | 0.542% |
| 3 | 5.087 | 541 | 544 | 558 | rVB | 567958 | 607135 | 2.06% | 0.393% |
| 4 | 5.298 | 576 | 580 | 584 | rBV | 450866 | 421655 | 1.43% | 0.273% |
| 5 | 5.757 | 654 | 658 | 662 | rVB | 1415343 | 1316836 | 4.46% | 0.852% |
| 6 | 6.016 | 694 | 702 | 705 | rBV | 317921 | 298826 | 1.01% | 0.193% |
| 7 | 6.093 | 712 | 715 | 722 | rVB | 330283 | 296215 | 1.00% | 0.192% |
| 8 | 6.151 | 722 | 725 | 728 | rBV | 679792 | 642804 | 2.18% | 0.416% |
| 9 | 6.263 | 742 | 744 | 748 | rVV | 708891 | 624871 | 2.12% | 0.404% |
| 10 | 6.322 | 750 | 754 | 757 | rVB | 974831 | 820603 | 2.78% | 0.531% |
| 11 | 6.434 | 769 | 773 | 780 | rVB | 675780 | 613349 | 2.08% | 0.397% |
| 12 | 6.516 | 780 | 787 | 790 | rBV2 | 1916192 | 2594088 | 8.79% | 1.679% |
| 13 | 6.557 | 790 | 794 | 796 | rVV | 579534 | 551773 | 1.87% | 0.357% |
| 14 | 6.581 | 796 | 798 | 801 | rVV | 521302 | 449197 | 1.52% | 0.291% |
| 15 | 6.622 | 801 | 805 | 807 | rVV | 360183 | 306278 | 1.04% | 0.198% |
| 16 | 6.669 | 807 | 813 | 818 | rVB3 | 2847941 | 3641142 | 12.33% | 2.357% |
| 17 | 7.057 | 872 | 879 | 883 | rBV3 | 499205 | 674001 | 2.28% | 0.436% |
| 18 | 7.457 | 942 | 947 | 953 | rBV | 739157 | 732795 | 2.48% | 0.474% |
| 19 | 7.522 | 953 | 958 | 962 | rVV2 | 475023 | 617274 | 2.09% | 0.400% |
| 20 | 7.592 | 968 | 970 | 973 | rVV | 691388 | 658968 | 2.23% | 0.426% |
| 21 | 7.757 | 995 | 998 | 1000 | rVV | 601384 | 653586 | 2.21% | 0.423% |
| 22 | 7.810 | 1000 | 1007 | 1010 | rVV2 | 4050407 | 5642150 | 19.11% | 3.652% |
| 23 | 7.857 | 1010 | 1015 | 1019 | rVB2 | 592828 | 595638 | 2.02% | 0.386% |
| 24 | 7.922 | 1023 | 1026 | 1028 | rBV | 546904 | 411440 | 1.39% | 0.266% |
| 25 | 7.963 | 1028 | 1033 | 1036 | rVV | 2103341 | 1932401 | 6.55% | 1.251% |
| 26 | 7.998 | 1036 | 1039 | 1041 | rVV | 601646 | 533774 | 1.81% | 0.345% |
| 27 | 8.039 | 1041 | 1046 | 1048 | rVV | 3004451 | 3133079 | 10.61% | 2.028% |
| 28 | 8.069 | 1048 | 1051 | 1054 | rVB | 1680033 | 1356957 | 4.60% | 0.878% |
| 29 | 8.175 | 1061 | 1069 | 1072 | rBV2 | 3847360 | 5770160 | 19.54% | 3.735% |
| 30 | 8.239 | 1072 | 1080 | 1082 | rVV | 1806147 | 2059447 | 6.98% | 1.333% |
| 31 | 8.263 | 1082 | 1084 | 1086 | rVV | 2327745 | 2211256 | 7.49% | 1.431% |
| 32 | 8.281 | 1086 | 1087 | 1094 | rVB2 | 1458462 | 1283588 | 4.35% | 0.831% |
| 33 | 8.375 | 1097 | 1103 | 1105 | rVV | 1612317 | 1504096 | 5.09% | 0.973% |
| 34 | 8.445 | 1112 | 1115 | 1116 | rVV | 535163 | 527578 | 1.79% | 0.341% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097074.D
Acq On : 26 Jul 2017 14:40
Operator : SJ/JU
Sample : I4443-05 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** E2-M7-ESW

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-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 8.463 | 1116 | 1118 | 1120 | rVV | 855746 | 944620 | 3.20% | 0.611% |
| 36 | 8.498 | 1120 | 1124 | 1126 | rVV2 | 1884159 | 2405786 | 8.15% | 1.557% |
| 37 | 8.534 | 1126 | 1130 | 1132 | rVV3 | 532151 | 734482 | 2.49% | 0.475% |
| 38 | 8.569 | 1134 | 1136 | 1138 | rVV | 1113082 | 928731 | 3.15% | 0.601% |
| 39 | 8.592 | 1138 | 1140 | 1145 | rVB2 | 1414607 | 1349988 | 4.57% | 0.874% |
| 40 | 8.657 | 1145 | 1151 | 1152 | rBV | 565874 | 520761 | 1.76% | 0.337% |
| 41 | 8.675 | 1152 | 1154 | 1160 | rVV3 | 1052922 | 1349656 | 4.57% | 0.874% |
| 42 | 8.734 | 1162 | 1164 | 1166 | rVV | 590216 | 582659 | 1.97% | 0.377% |
| 43 | 8.775 | 1169 | 1171 | 1174 | rVV2 | 661660 | 596696 | 2.02% | 0.386% |
| 44 | 8.857 | 1181 | 1185 | 1188 | rVB | 825324 | 704618 | 2.39% | 0.456% |
| 45 | 8.951 | 1198 | 1201 | 1208 | rVB5 | 301442 | 481460 | 1.63% | 0.312% |
| 46 | 9.192 | 1236 | 1242 | 1244 | rBV3 | 186965 | 306210 | 1.04% | 0.198% |
| 47 | 9.528 | 1293 | 1299 | 1302 | rBV | 987288 | 1098122 | 3.72% | 0.711% |
| 48 | 9.786 | 1337 | 1343 | 1350 | rVB2 | 991083 | 1379650 | 4.67% | 0.893% |
| 49 | 10.010 | 1378 | 1381 | 1384 | rBV | 431589 | 369558 | 1.25% | 0.239% |
| 50 | 10.310 | 1425 | 1432 | 1437 | rVV2 | 420790 | 567726 | 1.92% | 0.367% |
| 51 | 10.757 | 1493 | 1508 | 1511 | rBV | 3105914 | 7528429 | 25.50% | 4.873% |
| 52 | 10.998 | 1545 | 1549 | 1552 | rBV | 968791 | 860602 | 2.92% | 0.557% |
| 53 | 11.122 | 1565 | 1570 | 1572 | rBV2 | 581838 | 606422 | 2.05% | 0.392% |
| 54 | 11.527 | 1630 | 1639 | 1642 | rBV3 | 868228 | 2399118 | 8.13% | 1.553% |
| 55 | 11.651 | 1643 | 1660 | 1663 | rVB | 4665635 | 18376862 | 62.25% | 11.894% |
| 56 | 11.951 | 1708 | 1711 | 1713 | rVB | 356520 | 321461 | 1.09% | 0.208% |
| 57 | 11.992 | 1713 | 1718 | 1719 | rBV | 1261727 | 1195190 | 4.05% | 0.774% |
| 58 | 12.010 | 1719 | 1721 | 1724 | rVV | 897797 | 730725 | 2.48% | 0.473% |
| 59 | 12.257 | 1758 | 1763 | 1764 | rBV | 1692688 | 1851981 | 6.27% | 1.199% |
| 60 | 12.374 | 1764 | 1783 | 1785 | rVV5 | 5132836 | 29522612 | 100.00% | 19.108% |
| 61 | 12.427 | 1788 | 1792 | 1795 | rVV | 3430173 | 4952971 | 16.78% | 3.206% |
| 62 | 12.457 | 1795 | 1797 | 1800 | rVV2 | 1126114 | 1300536 | 4.41% | 0.842% |
| 63 | 12.492 | 1800 | 1803 | 1813 | rVV2 | 1092950 | 2142573 | 7.26% | 1.387% |
| 64 | 12.627 | 1821 | 1826 | 1828 | rVV | 1196844 | 1412659 | 4.79% | 0.914% |
| 65 | 12.704 | 1836 | 1839 | 1842 | rBV2 | 931269 | 993021 | 3.36% | 0.643% |
| 66 | 13.069 | 1889 | 1901 | 1905 | rBV2 | 2782167 | 7938178 | 26.89% | 5.138% |
| 67 | 13.145 | 1907 | 1914 | 1917 | rVB2 | 2158150 | 3705619 | 12.55% | 2.398% |
| 68 | 13.486 | 1969 | 1972 | 1974 | rVB | 418287 | 405126 | 1.37% | 0.262% |
| 69 | 13.639 | 1994 | 1998 | 2005 | rVB | 548961 | 800293 | 2.71% | 0.518% |
| 70 | 14.980 | 2222 | 2226 | 2232 | rBV | 431555 | 539087 | 1.83% | 0.349% |
| 71 | 15.598 | 2326 | 2331 | 2341 | rVB2 | 731226 | 1394082 | 4.72% | 0.902% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097074.D
Acq On : 26 Jul 2017 14:40
Operator : SJ/JU
Sample : I4443-05 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** E2-M7-ESW

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-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 72 | 16.692 | 2508 | 2517 | 2527 | rBV2 | 1178574 | 2879055 | 9.75% | 1.863% |
| 73 | 17.521 | 2650 | 2658 | 2668 | rVB2 | 435789 | 1069272 | 3.62% | 0.692% |

Sum of corrected areas: 154507942

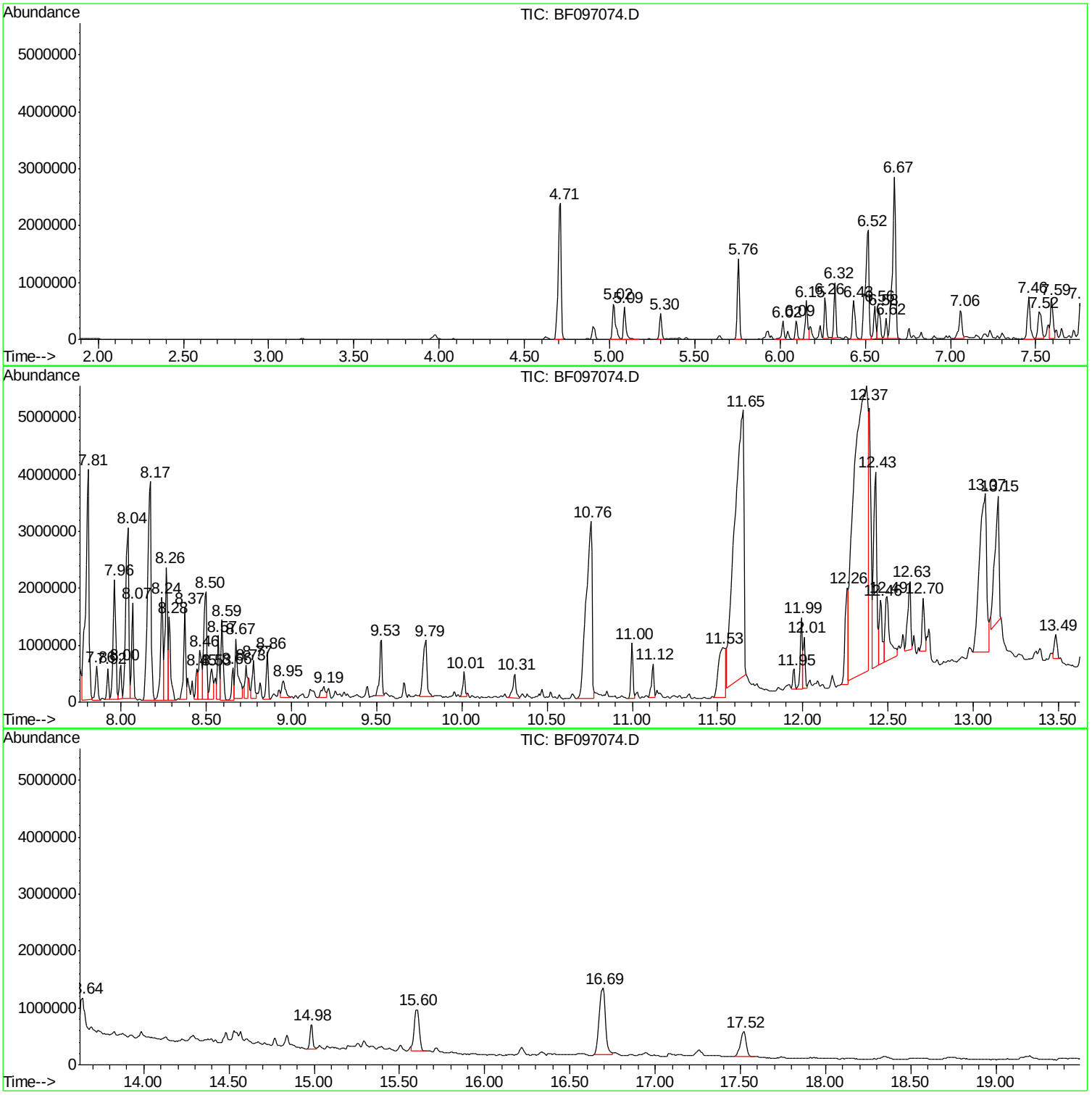
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097074.D
Acq On : 26 Jul 2017 14:40
Operator : SJ/JU
Sample : I4443-05 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** E2-M7-ESW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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\BF072617\
Data File : BF097074.D
Acq On : 26 Jul 2017 14:40
Operator : SJ/JU
Sample : I4443-05 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** E2-M7-ESW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

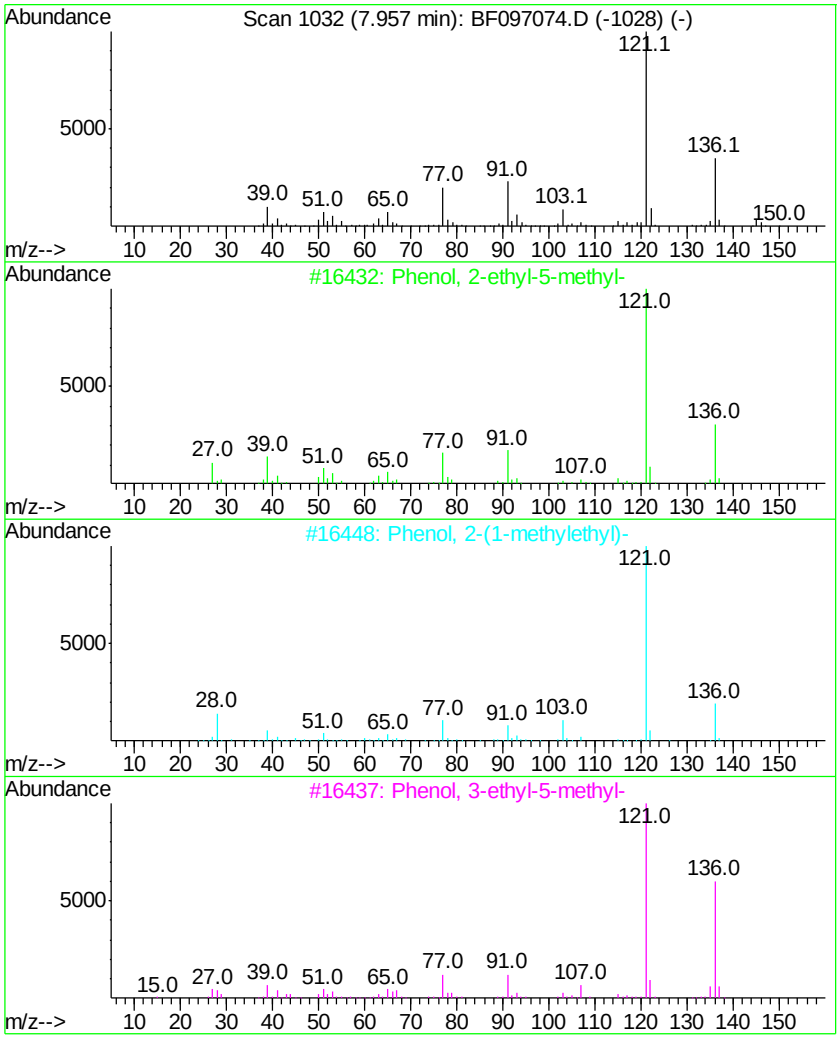
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

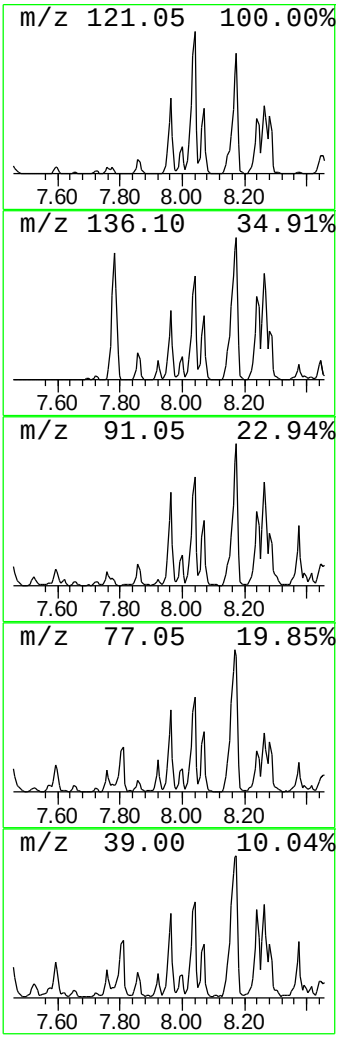
**********

Peak Number 1 Phenol, 2-ethyl-5-methyl- Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.96 | 59.13 ng | 1932400 | Naphthalene-d8 | 7.78 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenol, 2-ethyl-5-methyl- | 136 | C9H12O | 001687-61-2 | 90 |
| 2 | Phenol, 2-(1-methylethyl)- | 136 | C9H12O | 000088-69-7 | 86 |
| 3 | Phenol, 3-ethyl-5-methyl- | 136 | C9H12O | 000698-71-5 | 83 |
| 4 | Phenol, 4-(1-methylethyl)- | 136 | C9H12O | 000099-89-8 | 83 |
| 5 | Phenol, 3-(1-methylethyl)- | 136 | C9H12O | 000618-45-1 | 80 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097074.D
Acq On : 26 Jul 2017 14:40
Operator : SJ/JU
Sample : I4443-05 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** E2-M7-ESW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

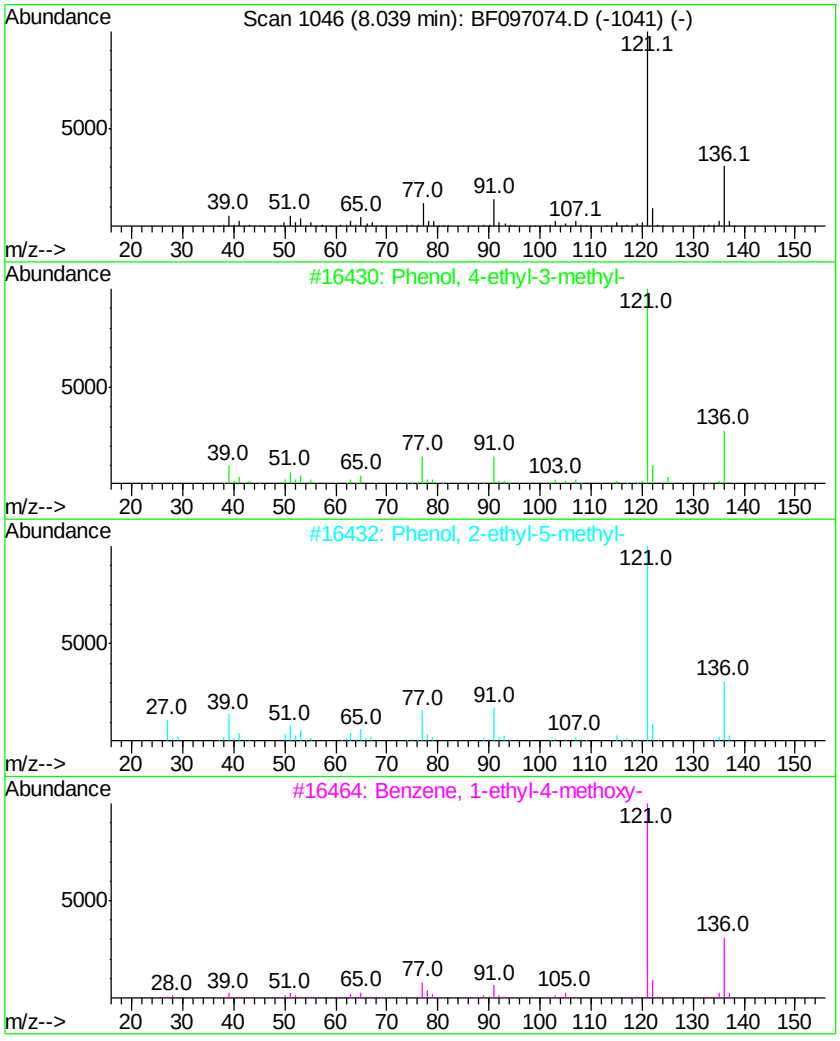
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

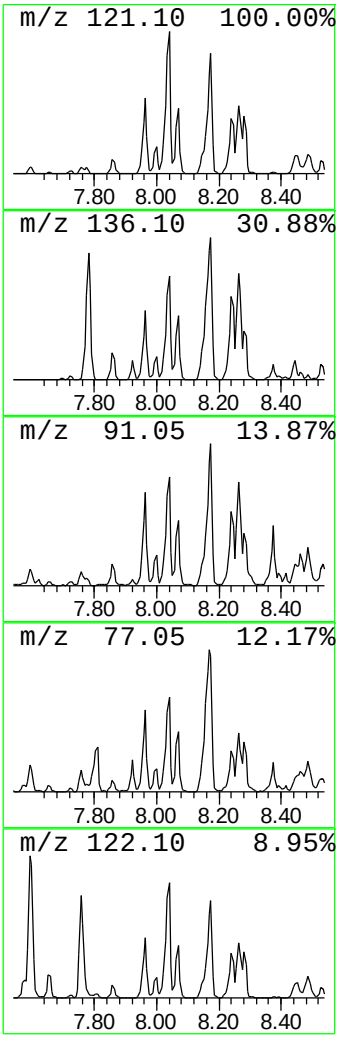
**********

Peak Number 2 Phenol, 4-ethyl-3-methyl- Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.04 | 95.87 ng | 3133080 | Naphthalene-d8 | 7.78 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenol, 4-ethyl-3-methyl- | 136 | C9H12O | 001123-94-0 | 94 |
| 2 | Phenol, 2-ethyl-5-methyl- | 136 | C9H12O | 001687-61-2 | 91 |
| 3 | Benzene, 1-ethyl-4-methoxy- | 136 | C9H12O | 001515-95-3 | 91 |
| 4 | Phenol, 2-(1-methylethyl)- | 136 | C9H12O | 000088-69-7 | 91 |
| 5 | Phenol, 2-ethyl-4-methyl- | 136 | C9H12O | 003855-26-3 | 90 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097074.D
Acq On : 26 Jul 2017 14:40
Operator : SJ/JU
Sample : I4443-05 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** E2-M7-ESW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

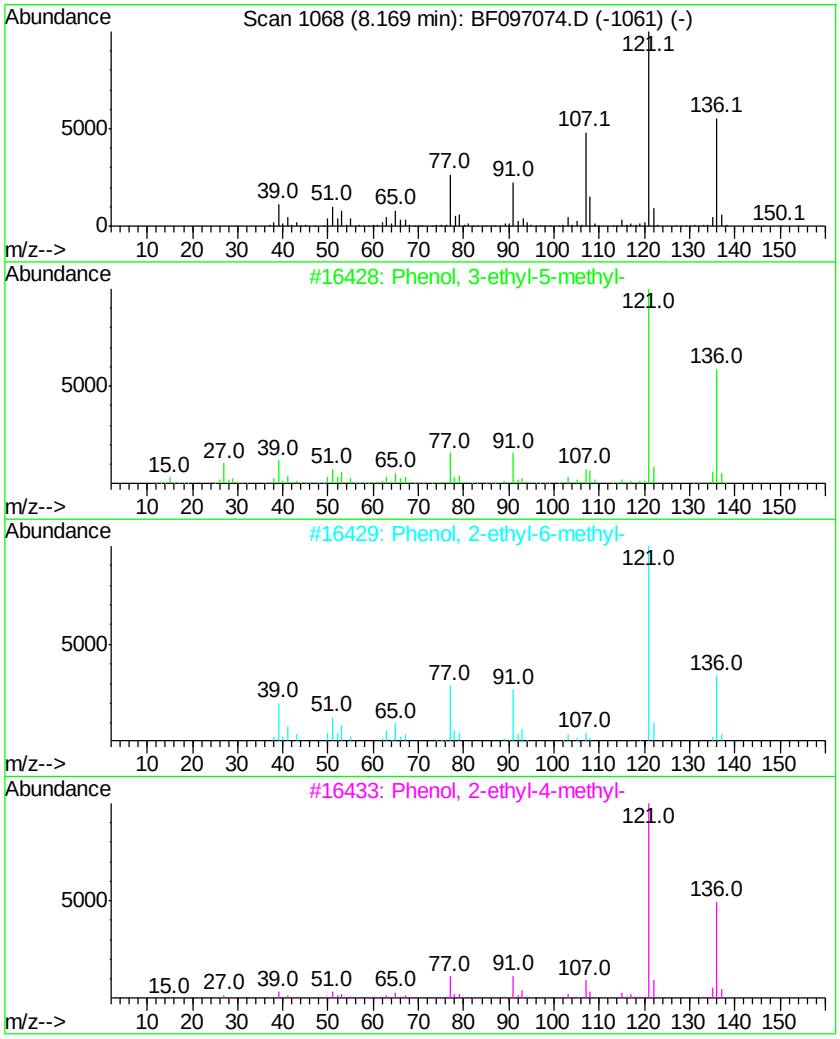
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

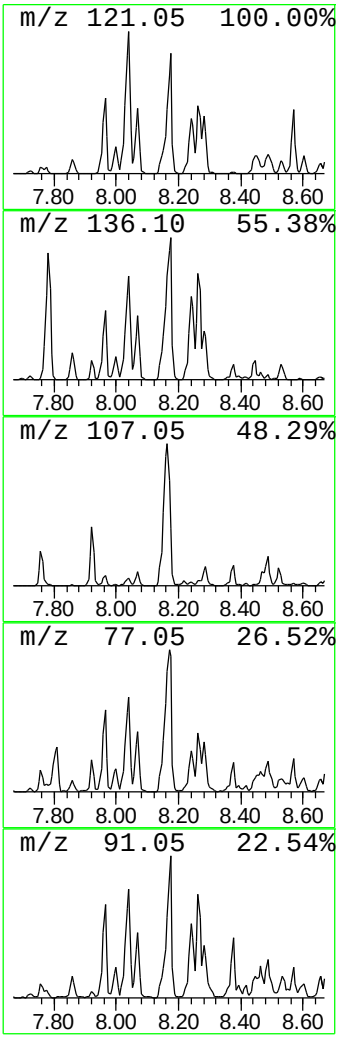
**********

Peak Number 4 Phenol, 3-ethyl-5-methyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.17 | 176.57 ng | 5770160 | Naphthalene-d8 | 7.78 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenol, 3-ethyl-5-methyl- | 136 | C9H12O | 000698-71-5 | 90 |
| 2 | Phenol, 2-ethyl-6-methyl- | 136 | C9H12O | 001687-64-5 | 87 |
| 3 | Phenol, 2-ethyl-4-methyl- | 136 | C9H12O | 003855-26-3 | 87 |
| 4 | Phenol, 3-(1-methylethyl)- | 136 | C9H12O | 000618-45-1 | 80 |
| 5 | Hydrazine, 1-(4-ethylphenyl)- | 136 | C8H12N2 | 054840-34-5 | 80 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097074.D
Acq On : 26 Jul 2017 14:40
Operator : SJ/JU
Sample : I4443-05 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** E2-M7-ESW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

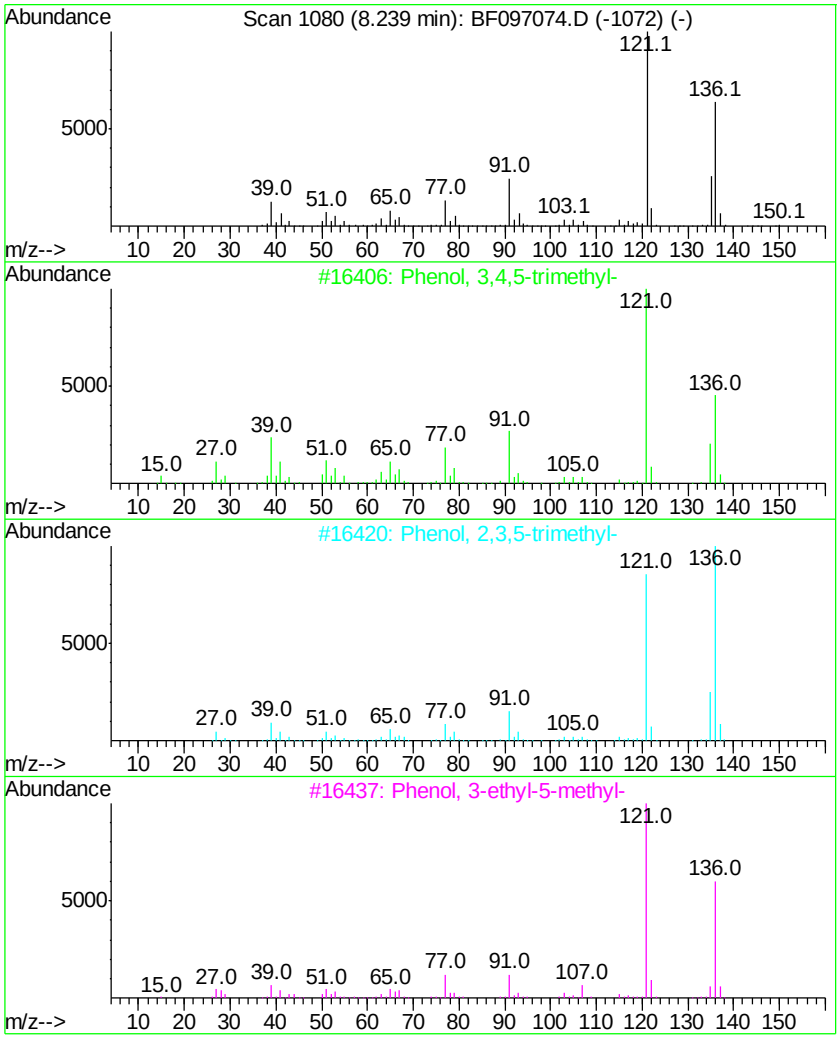
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

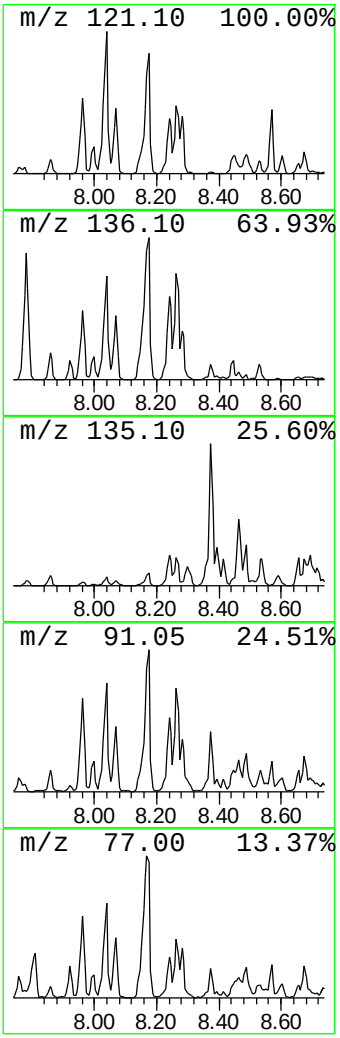
**********

Peak Number 5 Phenol, 3,4,5-trimethyl- Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.24 | 63.02 ng | 2059450 | Naphthalene-d8 | 7.78 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenol, 3,4,5-trimethyl- | 136 | C9H12O | 000527-54-8 | 91 |
| 2 | Phenol, 2,3,5-trimethyl- | 136 | C9H12O | 000697-82-5 | 90 |
| 3 | Phenol, 3-ethyl-5-methyl- | 136 | C9H12O | 000698-71-5 | 90 |
| 4 | Phenol, 3,4,5-trimethyl-, methyl... | 193 | C11H15NO2 | 002686-99-9 | 90 |
| 5 | Phenol, 2,4,5-trimethyl- | 136 | C9H12O | 000496-78-6 | 87 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097074.D
Acq On : 26 Jul 2017 14:40
Operator : SJ/JU
Sample : I4443-05 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** E2-M7-ESW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

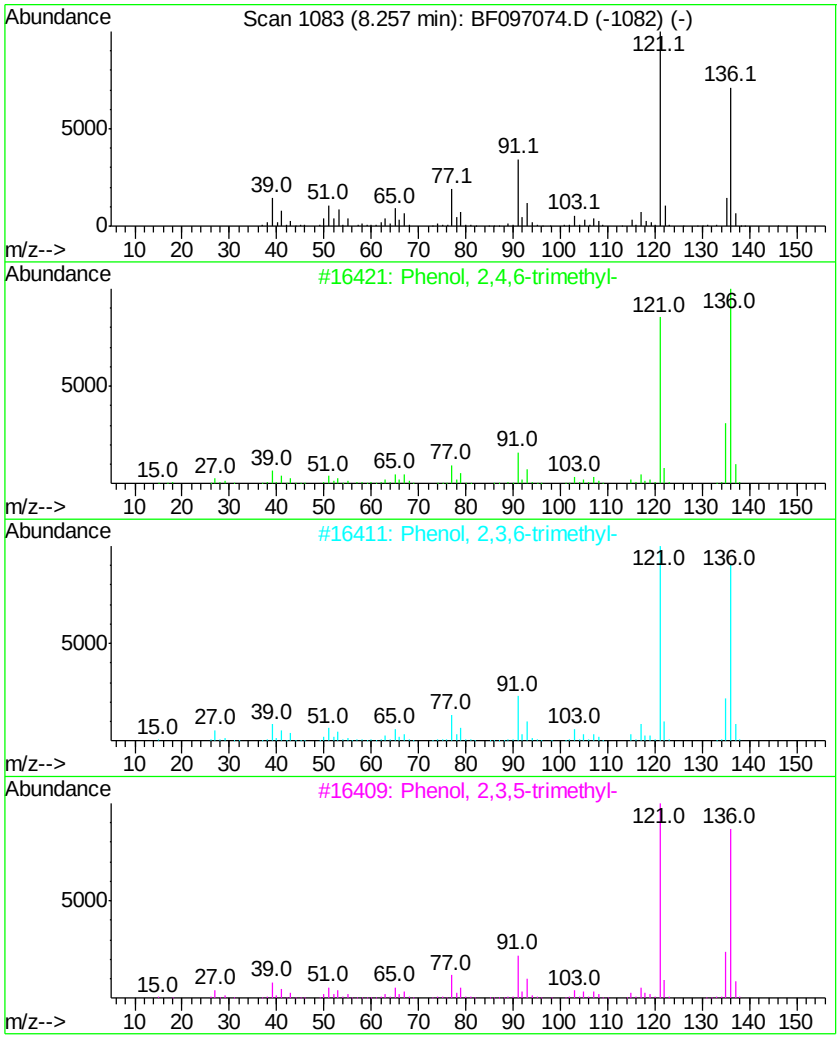
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

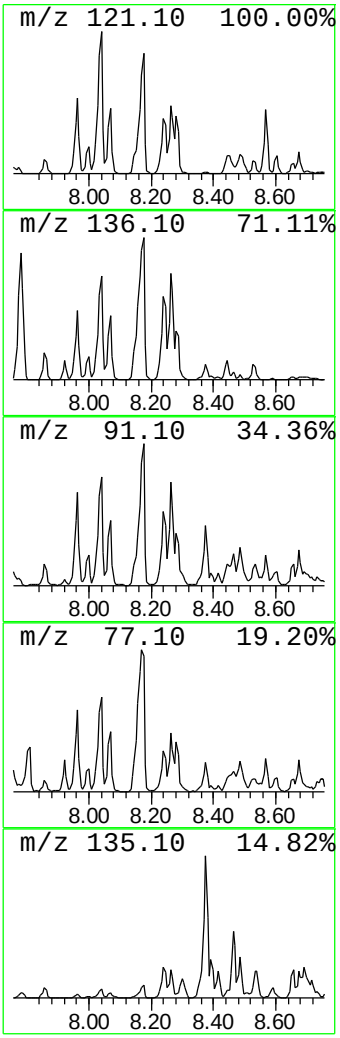
**********

Peak Number 6 Phenol, 2,4,6-trimethyl- Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.26 | 67.67 ng | 2211260 | Naphthalene-d8 | 7.78 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenol, 2,4,6-trimethyl- | 136 | C9H12O | 000527-60-6 | 97 |
| 2 | Phenol, 2,3,6-trimethyl- | 136 | C9H12O | 002416-94-6 | 97 |
| 3 | Phenol, 2,3,5-trimethyl- | 136 | C9H12O | 000697-82-5 | 96 |
| 4 | Phenol, 3,4,5-trimethyl- | 136 | C9H12O | 000527-54-8 | 94 |
| 5 | Phenol, 2,4,5-trimethyl- | 136 | C9H12O | 000496-78-6 | 94 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097074.D
Acq On : 26 Jul 2017 14:40
Operator : SJ/JU
Sample : I4443-05 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** E2-M7-ESW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

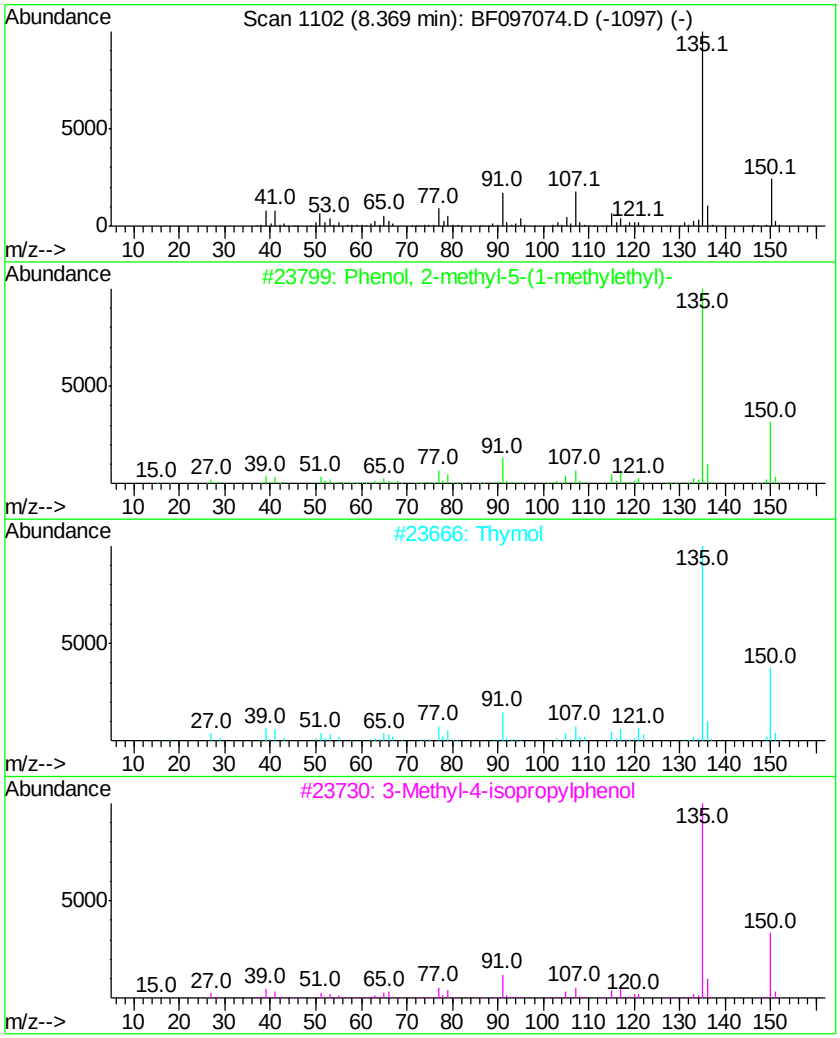
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

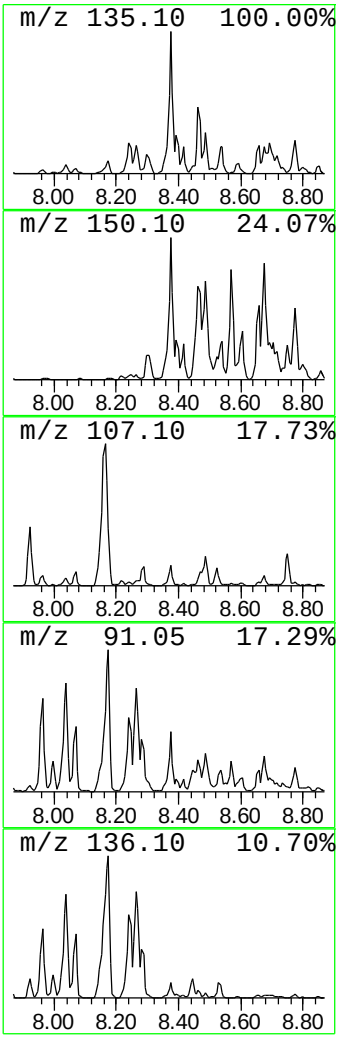
**********

Peak Number 7 Phenol, 2-methyl-5-(1-methy... Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.37 | 46.03 ng | 1504100 | Naphthalene-d8 | 7.78 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Phenol, 2-methyl-5-(1-methylethyl)- | 150 | C10H14O | 000499-75-2 | 91 |
| 2 | Thymol | 150 | C10H14O | 000089-83-8 | 91 |
| 3 | 3-Methyl-4-isopropylphenol | 150 | C10H14O | 003228-02-2 | 90 |
| 4 | Benzene, 1-methoxy-4-(1-methylet... | 150 | C10H14O | 004132-48-3 | 80 |
| 5 | 4-Acetylanisole | 150 | C9H10O2 | 000100-06-1 | 80 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097074.D
Acq On : 26 Jul 2017 14:40
Operator : SJ/JU
Sample : I4443-05 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** E2-M7-ESW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

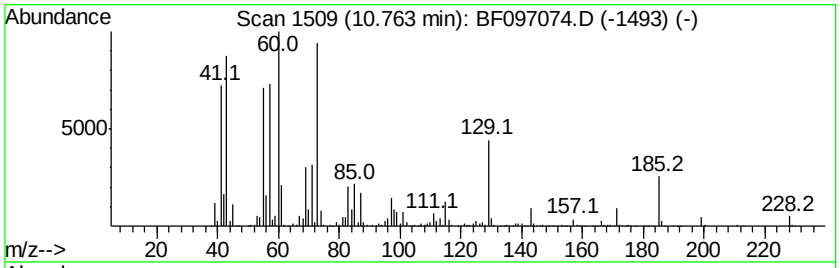
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

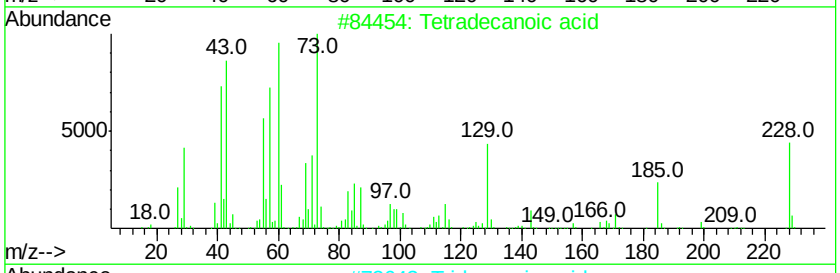
**********

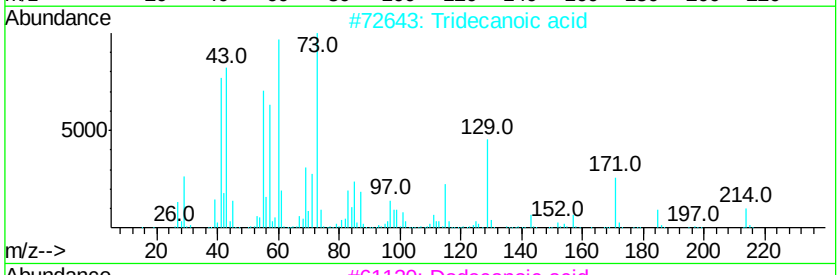
Peak Number 9 Tetradecanoic acid Concentration Rank 5

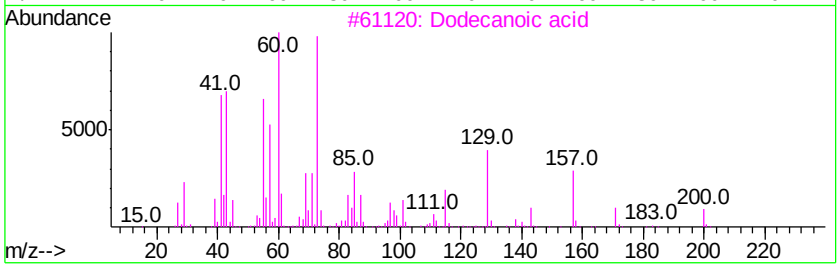
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.76 | 174.96 ng | 7528430 | Phenanthrene-d10 | 11.00 |

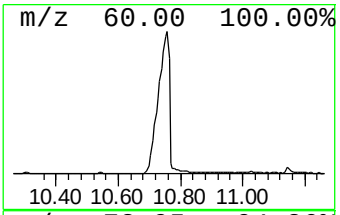
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 94 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 87 |
| 3 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 72 |
| 4 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 53 |
| 5 | Undecanoic acid, 10-bromo- | 264 | C11H21BrO2 | 018294-93-4 | 47 |

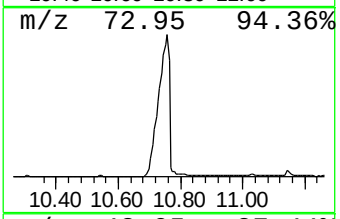


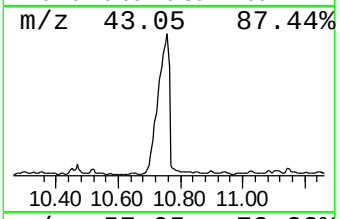



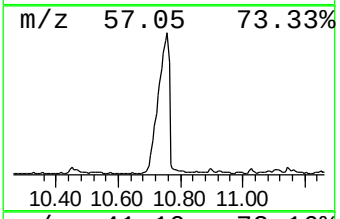



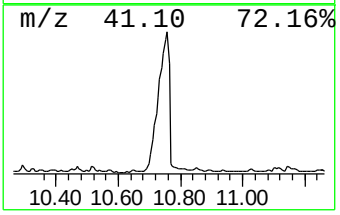



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097074.D
Acq On : 26 Jul 2017 14:40
Operator : SJ/JU
Sample : I4443-05 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** E2-M7-ESW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

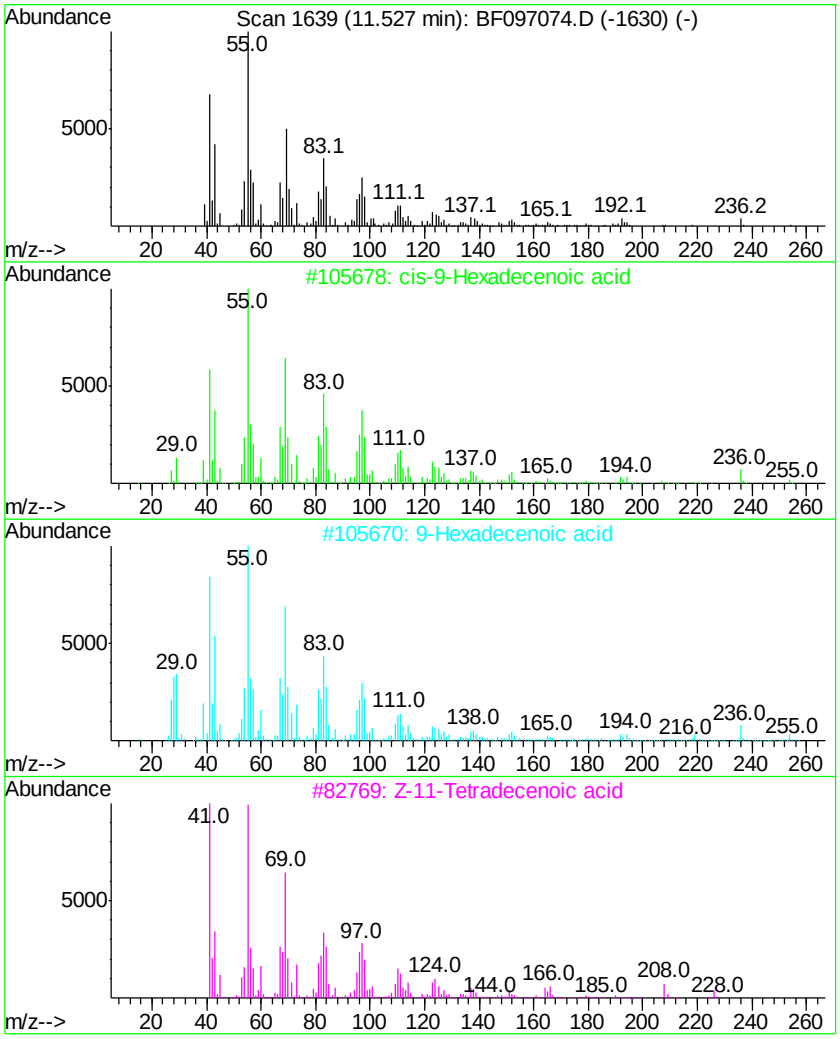
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

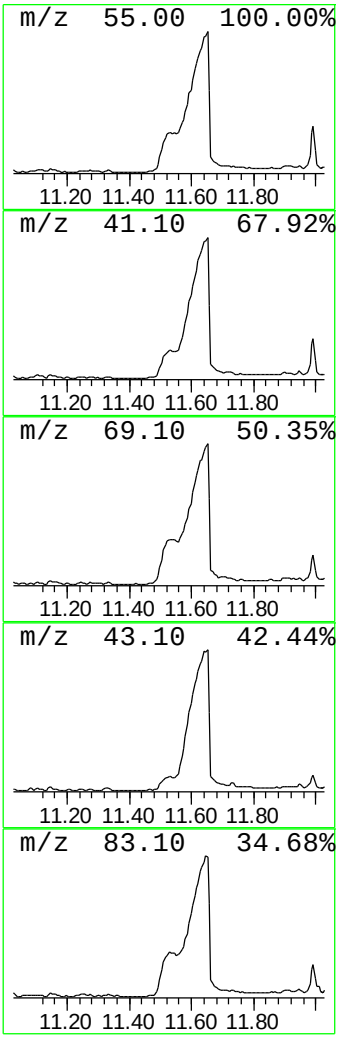
**********

Peak Number 10 cis-9-Hexadecenoic acid Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.53 | 55.75 ng | 2399120 | Phenanthrene-d10 | 11.00 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | cis-9-Hexadecenoic acid | 254 | C16H30O2 | 1000333-19-5 | 91 |
| 2 | 9-Hexadecenoic acid | 254 | C16H30O2 | 002091-29-4 | 91 |
| 3 | Z-11-Tetradecenoic acid | 226 | C14H26O2 | 1000130-83-3 | 90 |
| 4 | Oxacycloheptadecan-2-one | 254 | C16H30O2 | 000109-29-5 | 90 |
| 5 | Hexadecenoic acid, Z-11- | 254 | C16H30O2 | 002416-20-8 | 90 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097074.D
Acq On : 26 Jul 2017 14:40
Operator : SJ/JU
Sample : I4443-05 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** E2-M7-ESW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

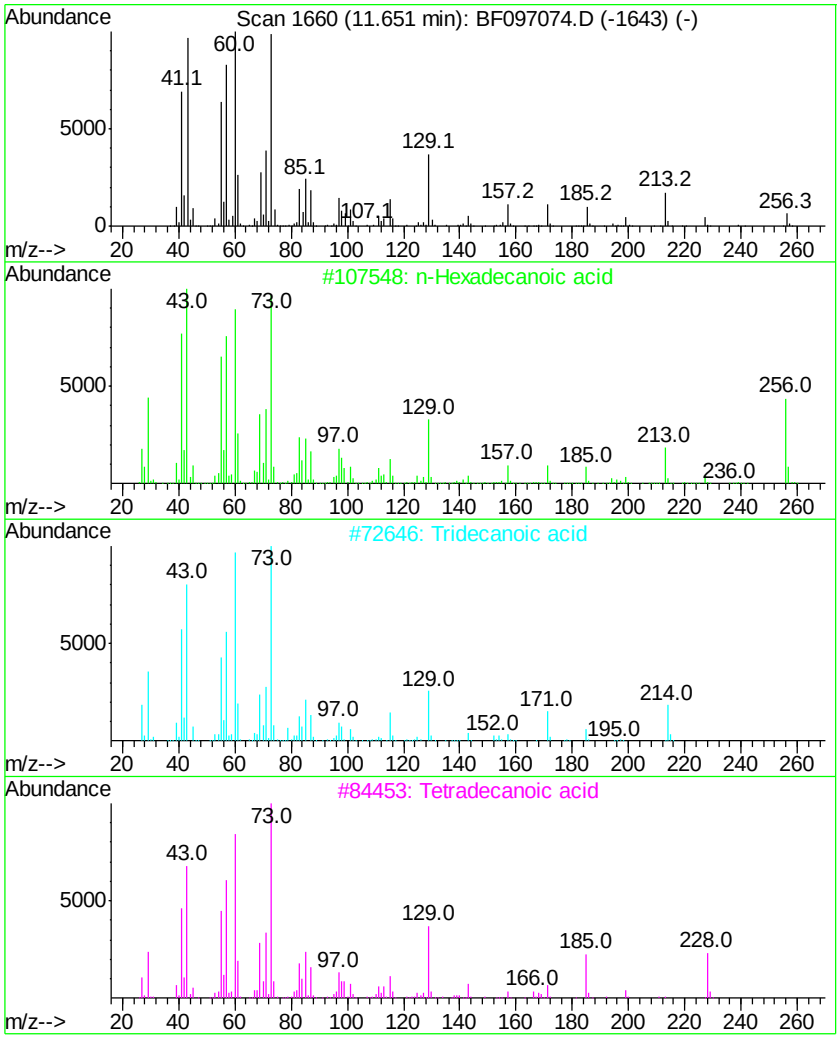
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

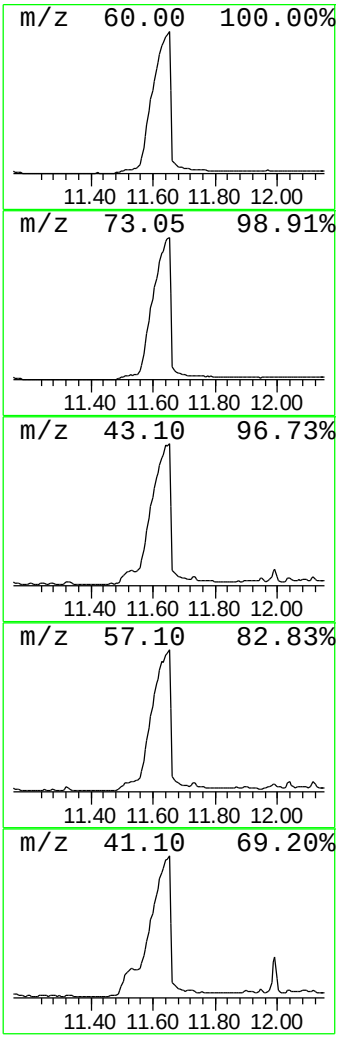
**********

Peak Number 11 n-Hexadecanoic acid Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.65 | 427.07 ng | 18376900 | Phenanthrene-d10 | 11.00 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 83 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 80 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 80 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 78 |
| 5 | Methyl 2,6-anhydro-.alpha.-d-alt... | 176 | C7H12O5 | 1000130-02-0 | 22 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097074.D
Acq On : 26 Jul 2017 14:40
Operator : SJ/JU
Sample : I4443-05 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** E2-M7-ESW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

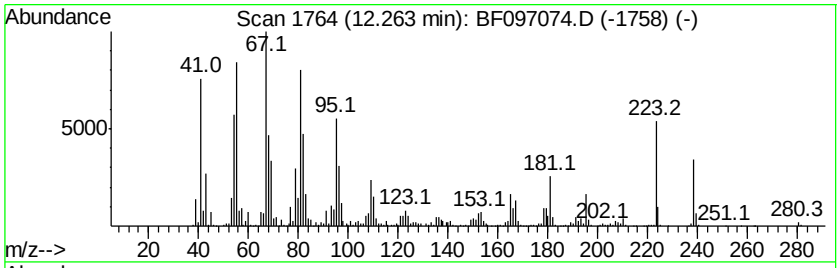
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

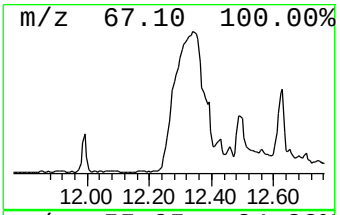
**********

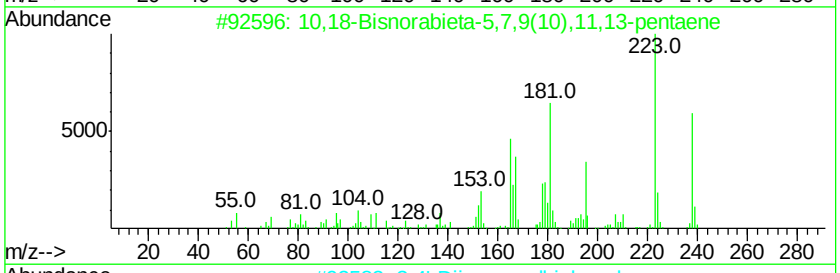
Peak Number 12 10,18-Bisnorabieta-5,7,9(10... Concentration Rank 17

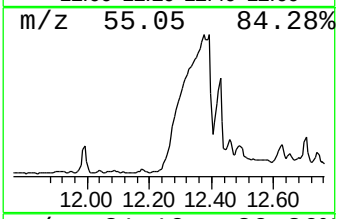
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.26 | 43.04 ng | 1851980 | Phenanthrene-d10 | 11.00 |

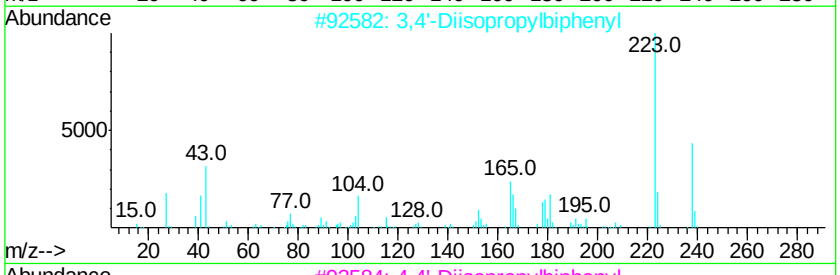
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 10,18-Bisnorabieta-5,7,9(10),11,... | 238 | C18H22 | 006566-19-4 | 99 |
| 2 | 3,4'-Diisopropylbiphenyl | 238 | C18H22 | 061434-46-6 | 60 |
| 3 | 4,4'-Diisopropylbiphenyl | 238 | C18H22 | 018970-30-4 | 50 |
| 4 | 3,3'-Diacetylbiphenyl | 238 | C16H14O2 | 094113-07-2 | 50 |
| 5 | 2-Propenoic acid, 3-(3,4,5-trime... | 238 | C12H14O5 | 000090-50-6 | 45 |

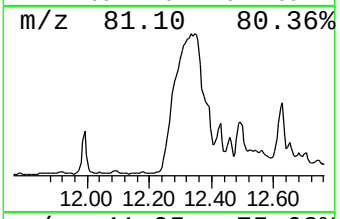


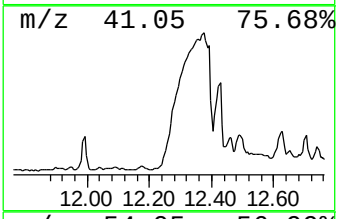



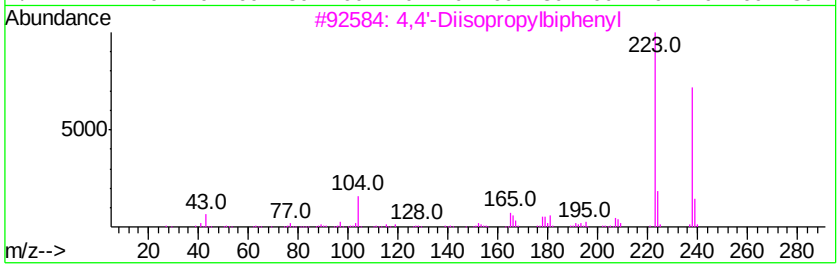



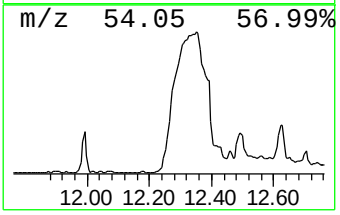



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097074.D
Acq On : 26 Jul 2017 14:40
Operator : SJ/JU
Sample : I4443-05 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** E2-M7-ESW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

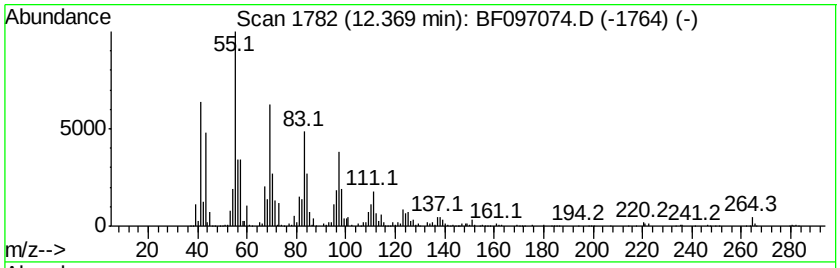
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

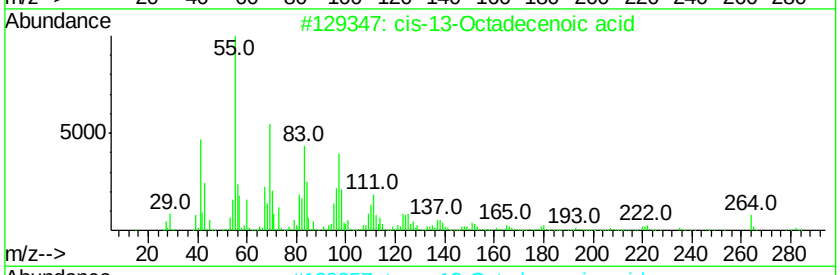
**********

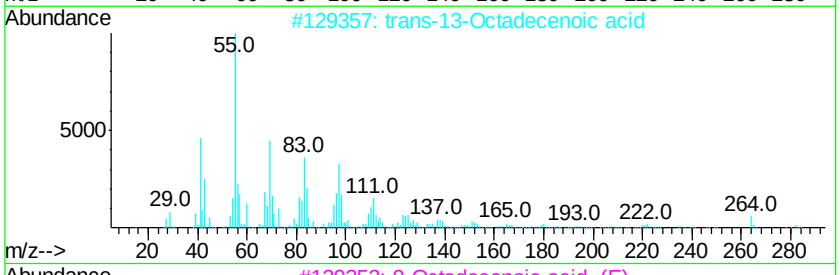
Peak Number 13 cis-13-Octadecenoic acid Concentration Rank 1

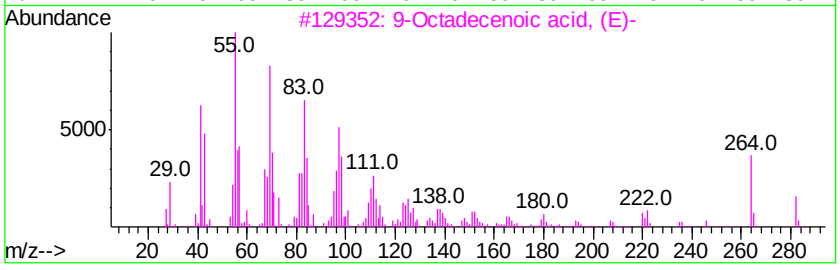
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.37 | 737.80 ng | 29522600 | Chrysene-d12 | 13.63 |

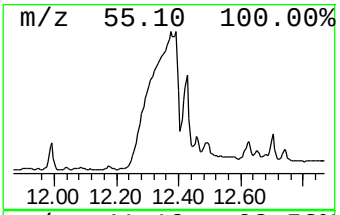
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | cis-13-Octadecenoic acid | 282 | C18H34O2 | 013126-39-1 | 91 |
| 2 | trans-13-Octadecenoic acid | 282 | C18H34O2 | 000693-71-0 | 83 |
| 3 | 9-Octadecenoic acid, (E)- | 282 | C18H34O2 | 000112-79-8 | 74 |
| 4 | cis-Vaccenic acid | 282 | C18H34O2 | 000506-17-2 | 64 |
| 5 | 6-Octadecenoic acid, (Z)- | 282 | C18H34O2 | 000593-39-5 | 64 |

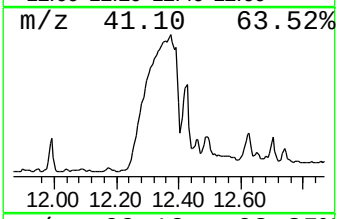


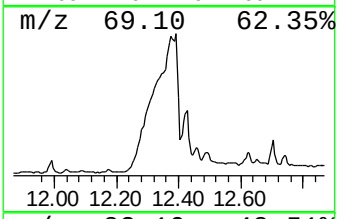



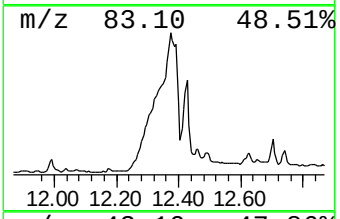



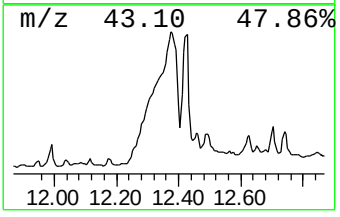



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097074.D
Acq On : 26 Jul 2017 14:40
Operator : SJ/JU
Sample : I4443-05 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** E2-M7-ESW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

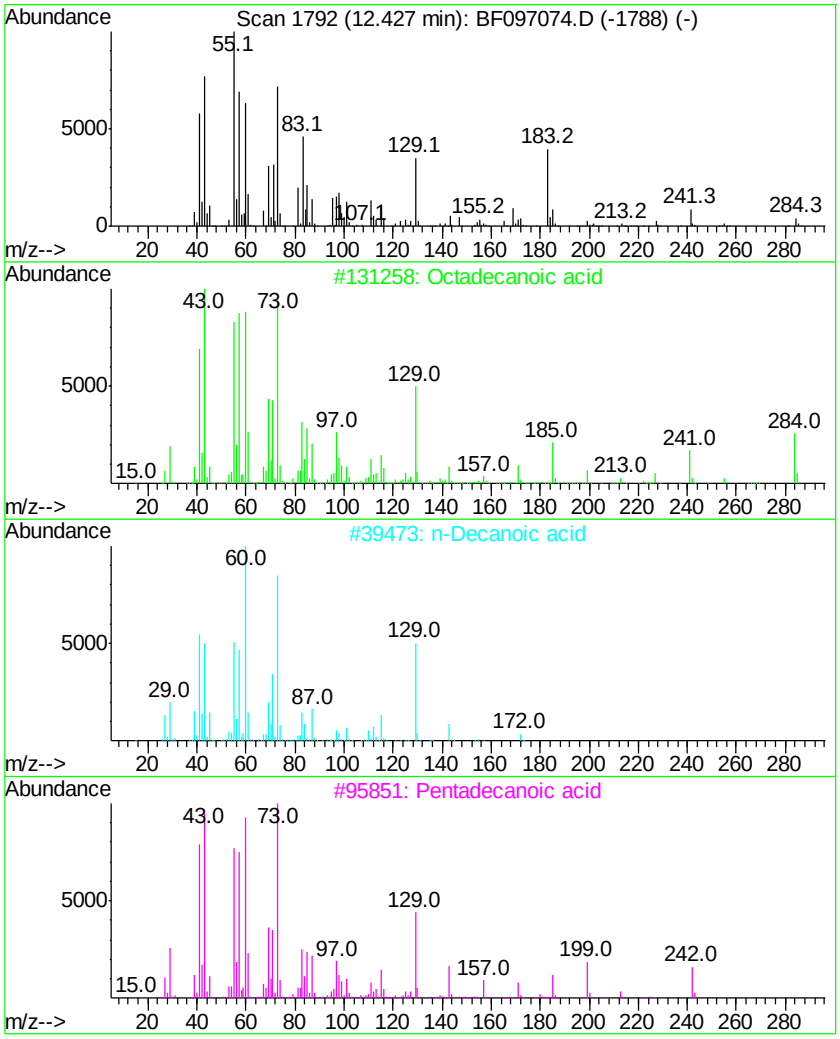
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

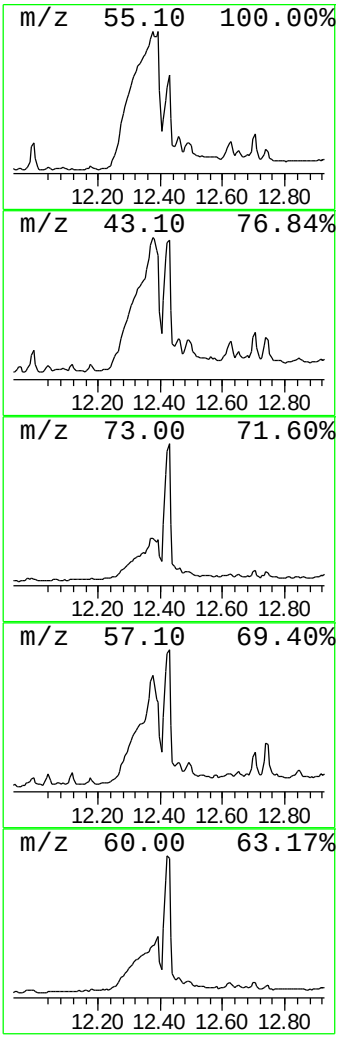
**********

Peak Number 14 Octadecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.43 | 123.78 ng | 4952970 | Chrysene-d12 | 13.63 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 97 |
| 2 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 70 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 45 |
| 4 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 45 |
| 5 | Ethanone, 1-(4,5-dihydro-2-thiaz... | 129 | C5H7NOS | 029926-41-8 | 38 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097074.D
Acq On : 26 Jul 2017 14:40
Operator : SJ/JU
Sample : I4443-05 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** E2-M7-ESW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

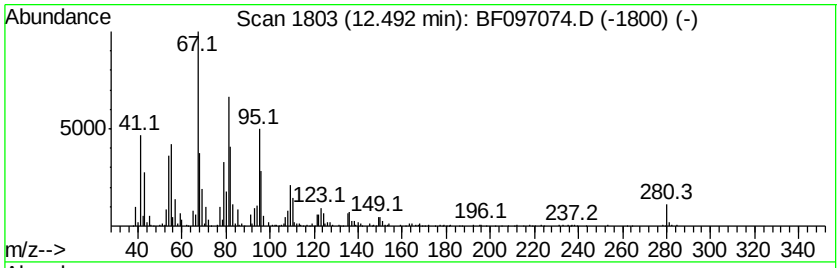
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

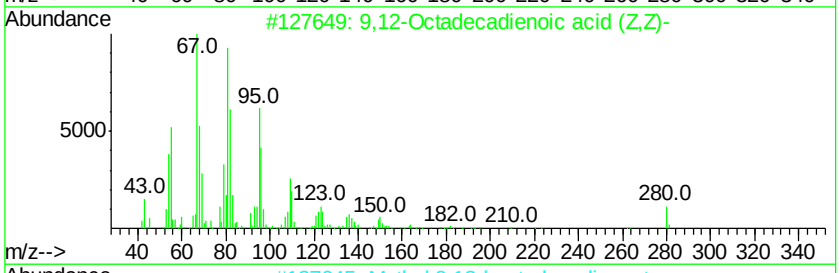
**********

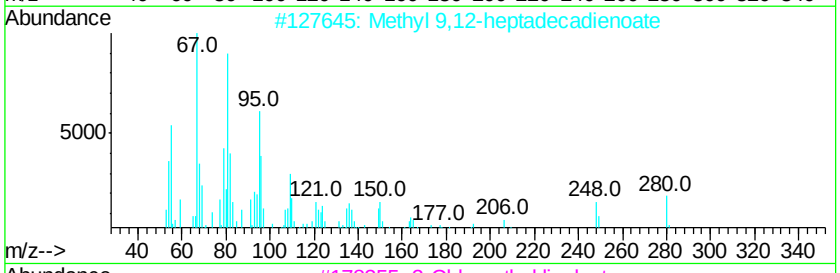
Peak Number 15 9,12-Octadecadienoic acid (... Concentration Rank 14

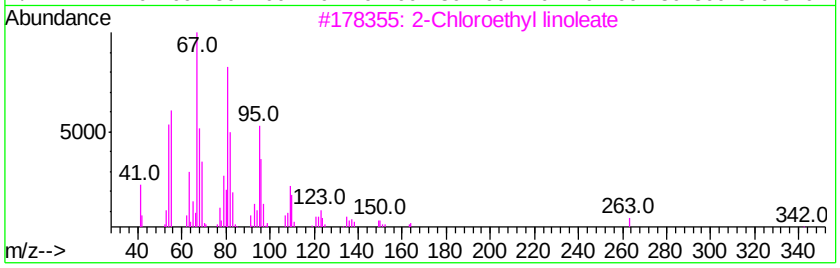
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.49 | 53.54 ng | 2142570 | Chrysene-d12 | 13.63 |

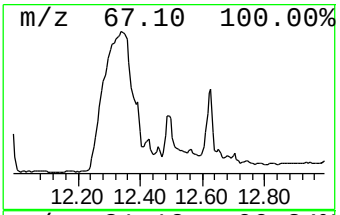
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9,12-Octadecadienoic acid (Z,Z)- | 280 | C18H32O2 | 000060-33-3 | 96 |
| 2 | Methyl 9,12-heptadecadienoate | 280 | C18H32O2 | 1000336-36-2 | 90 |
| 3 | 2-Chloroethyl linoleate | 342 | C20H35ClO2 | 025525-76-2 | 90 |
| 4 | 9,12-Octadecadienoic acid, methy... | 294 | C19H34O2 | 002566-97-4 | 87 |
| 5 | 9,17-Octadecadienal, (Z)- | 264 | C18H32O | 056554-35-9 | 86 |

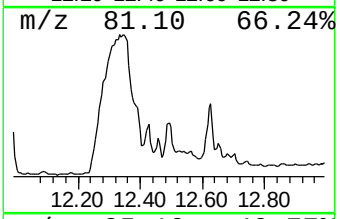


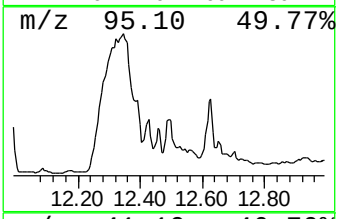



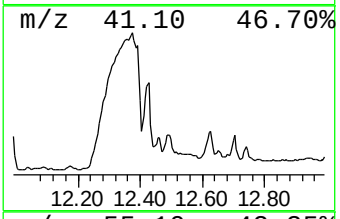



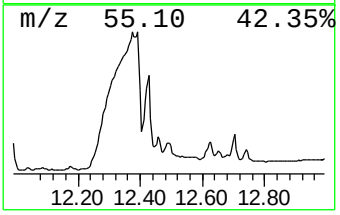



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097074.D
Acq On : 26 Jul 2017 14:40
Operator : SJ/JU
Sample : I4443-05 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** E2-M7-ESW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

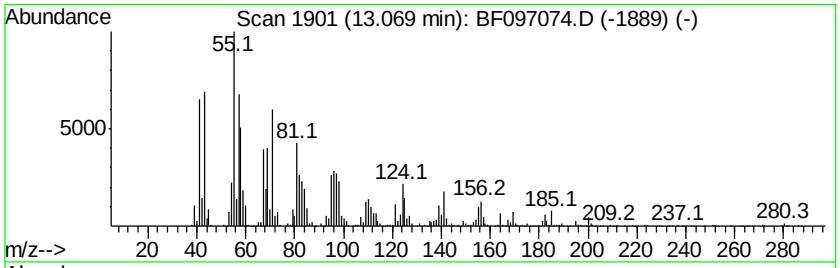
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

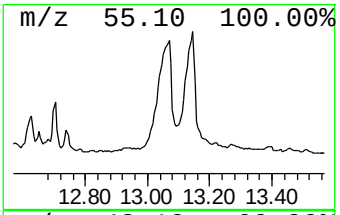
**********

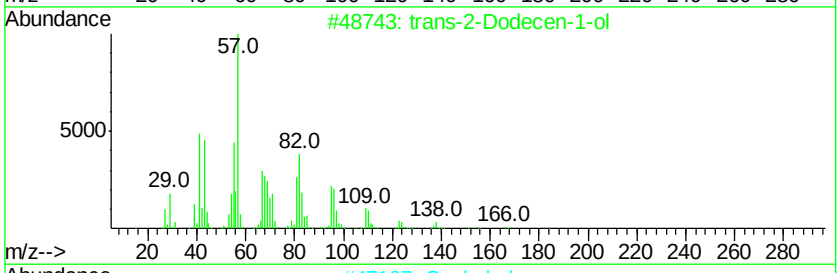
Peak Number 16 unknown13.07 Concentration Rank 3

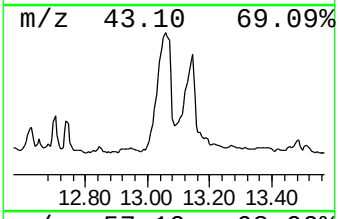
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.07 | 198.38 ng | 7938180 | Chrysene-d12 | 13.63 |

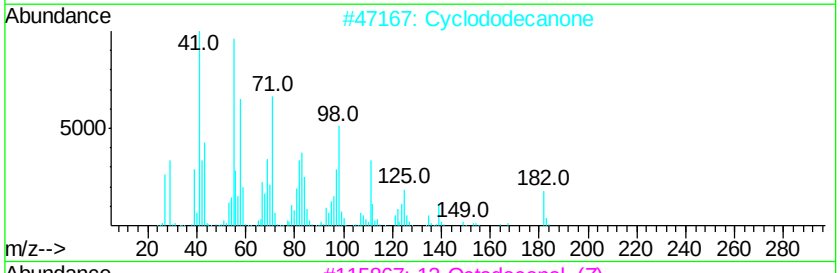
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | trans-2-Dodecen-1-ol | 184 | C12H24O | 069064-37-5 | 46 |
| 2 | Cyclododecanone | 182 | C12H22O | 000830-13-7 | 45 |
| 3 | 13-Octadecenal, (Z)- | 266 | C18H34O | 058594-45-9 | 43 |
| 4 | cis-7,cis-11-Hexadecadien-1-yl a... | 280 | C18H32O2 | 052207-99-5 | 38 |
| 5 | 13-Tetradecenal | 210 | C14H26O | 085896-31-7 | 38 |

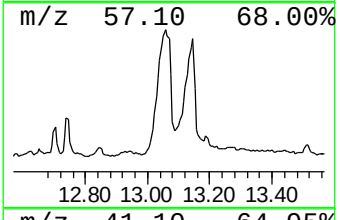


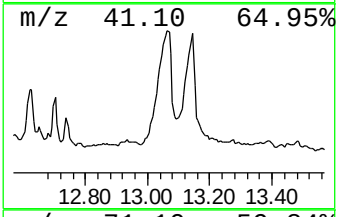



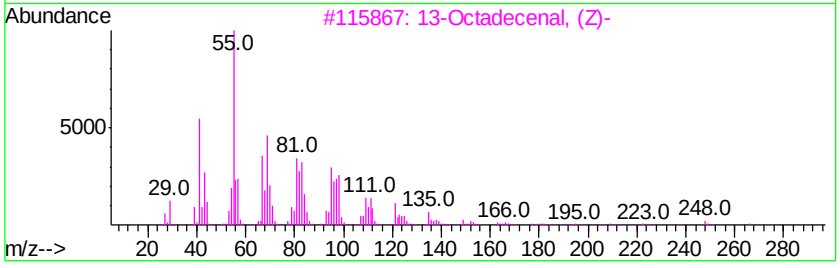



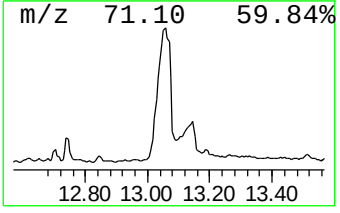



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097074.D
Acq On : 26 Jul 2017 14:40
Operator : SJ/JU
Sample : I4443-05 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** E2-M7-ESW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

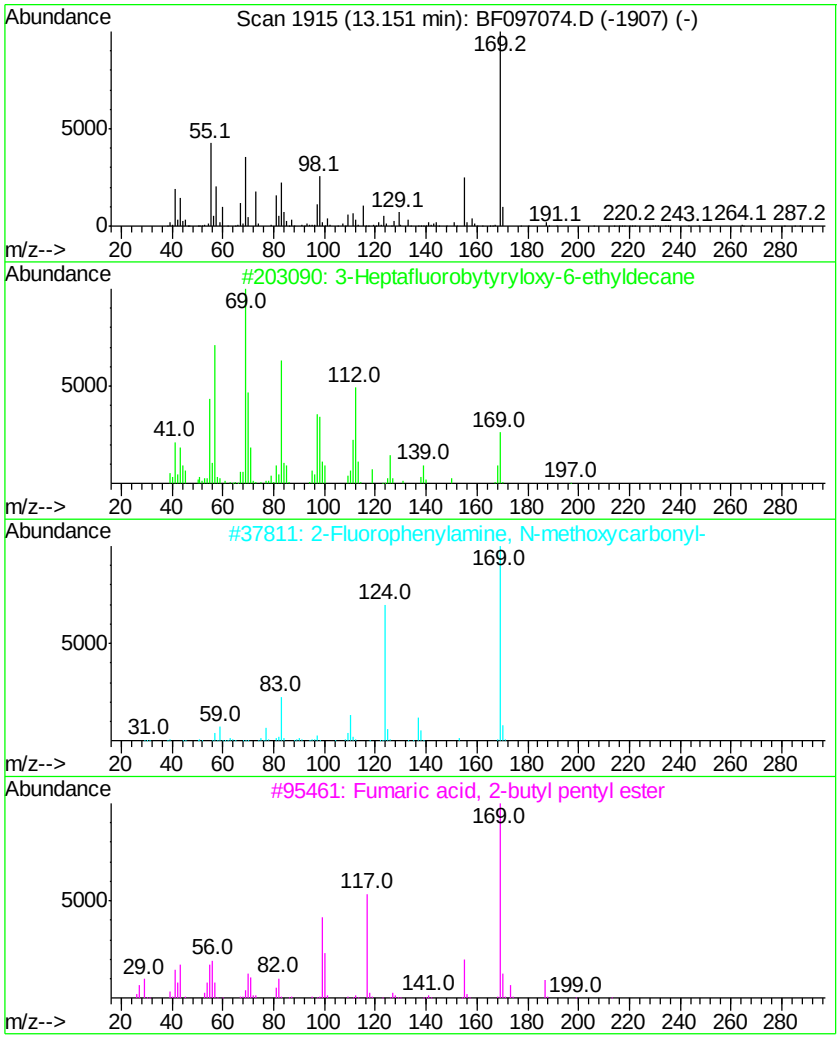
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

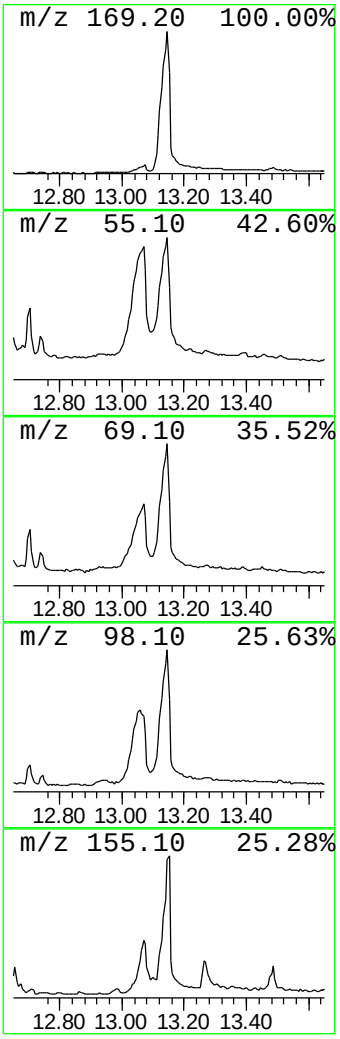
**********

Peak Number 17 unknown13.15 Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.15 | 92.61 ng | 3705620 | Chrysene-d12 | 13.63 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Heptafluorobytyryloxy-6-ethyld... | 382 | C16H25F7O2 | 1000215-97-2 | 38 |
| 2 | 2-Fluorophenylamine, N-methoxyca... | 169 | C8H8FNO2 | 1000343-97-8 | 38 |
| 3 | Fumaric acid, 2-butyl pentyl ester | 242 | C13H22O4 | 1000348-64-1 | 35 |
| 4 | [1,1'-Biphenyl]-2-amine | 169 | C12H11N | 000090-41-5 | 25 |
| 5 | 4-Pyridinol, 2,6-dimethyl-3-[met... | 169 | C8H11NOS | 1000251-72-8 | 25 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097074.D
Acq On : 26 Jul 2017 14:40
Operator : SJ/JU
Sample : I4443-05 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** E2-M7-ESW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

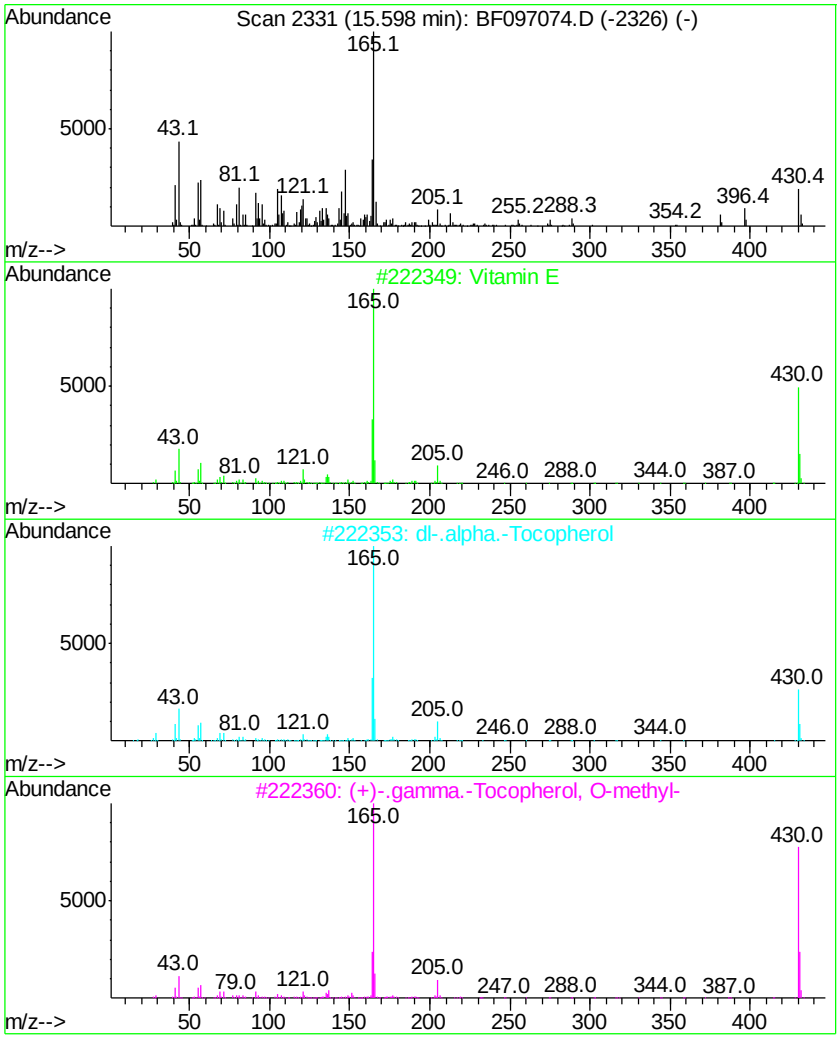
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

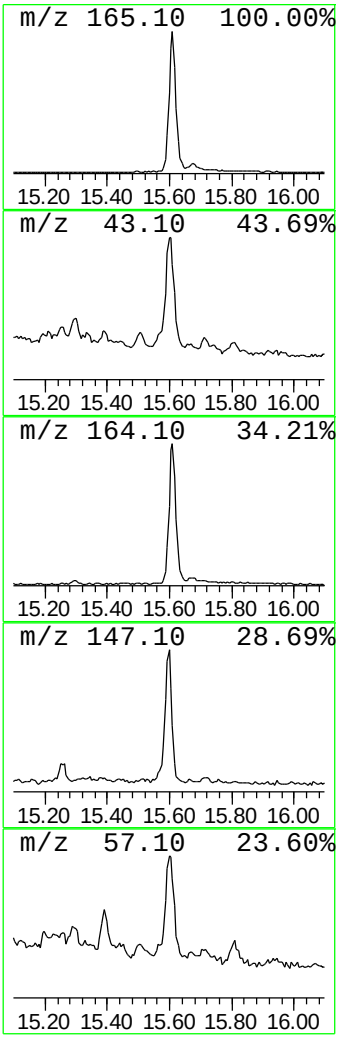
**********

Peak Number 18 Vitamin E Concentration Rank 15

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.60 | 51.72 ng | 1394080 | Perylene-d12 | 14.98 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Vitamin E | 430 | C29H50O2 | 000059-02-9 | 95 |
| 2 | dl-.alpha.-Tocopherol | 430 | C29H50O2 | 010191-41-0 | 94 |
| 3 | (+)-.gamma.-Tocopherol, O-methyl- | 430 | C29H50O2 | 1000374-72-2 | 76 |
| 4 | 1-(m-Dimethylaminophenyl)ethanol | 165 | C10H15NO | 005339-01-5 | 52 |
| 5 | 1H-Purin-2-amine, 6-methoxy- | 165 | C6H7N5O | 020535-83-5 | 49 |



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097074.D
Acq On : 26 Jul 2017 14:40
Operator : SJ/JU
Sample : I4443-05 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** E2-M7-ESW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

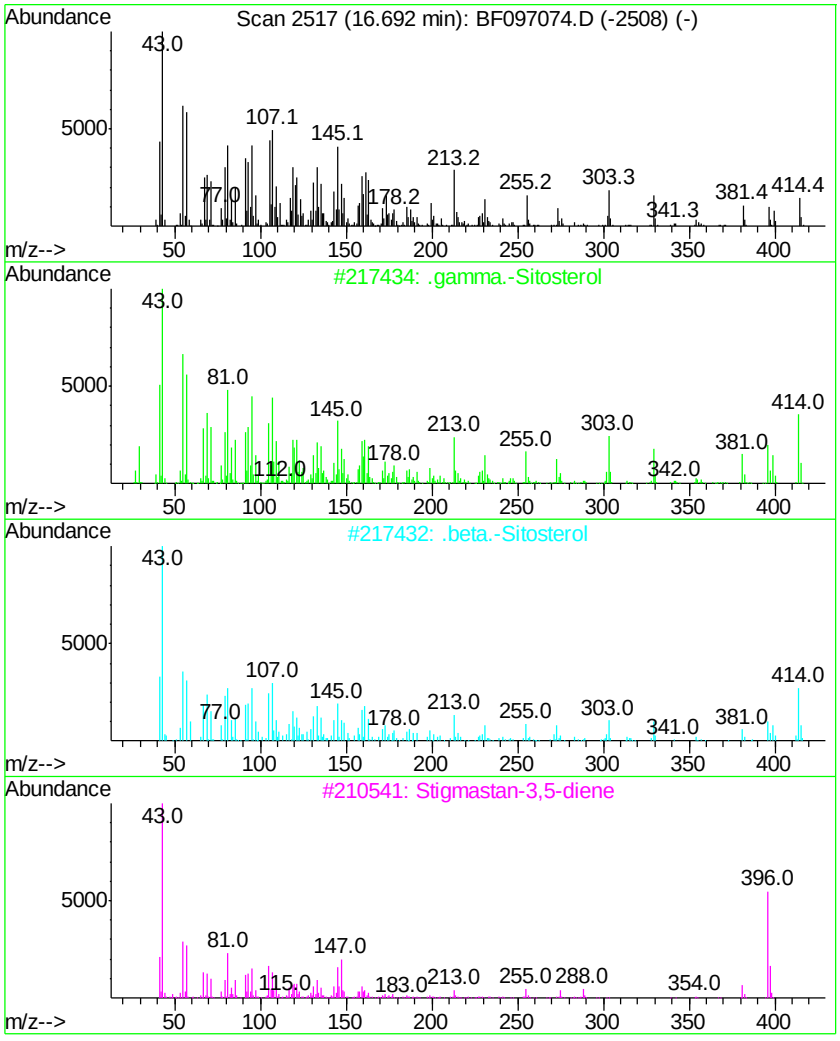
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

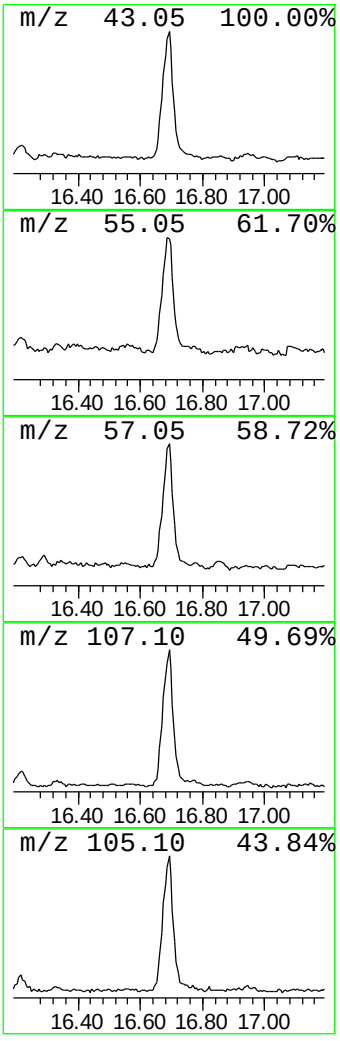
**********

Peak Number 19 .gamma.-Sitosterol Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.69 | 106.81 ng | 2879060 | Perylene-d12 | 14.98 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | .gamma.-Sitosterol | 414 | C29H50O | 000083-47-6 | 99 |
| 2 | .beta.-Sitosterol | 414 | C29H50O | 000083-46-5 | 96 |
| 3 | Stigmastan-3,5-diene | 396 | C29H48 | 1000214-16-4 | 60 |
| 4 | Isocholesteryl methyl ether | 400 | C28H48O | 029944-53-4 | 53 |
| 5 | Ergost-5-en-3-ol, (3.beta.)- | 400 | C28H48O | 004651-51-8 | 50 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097074.D
Acq On : 26 Jul 2017 14:40
Operator : SJ/JU
Sample : I4443-05 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** E2-M7-ESW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

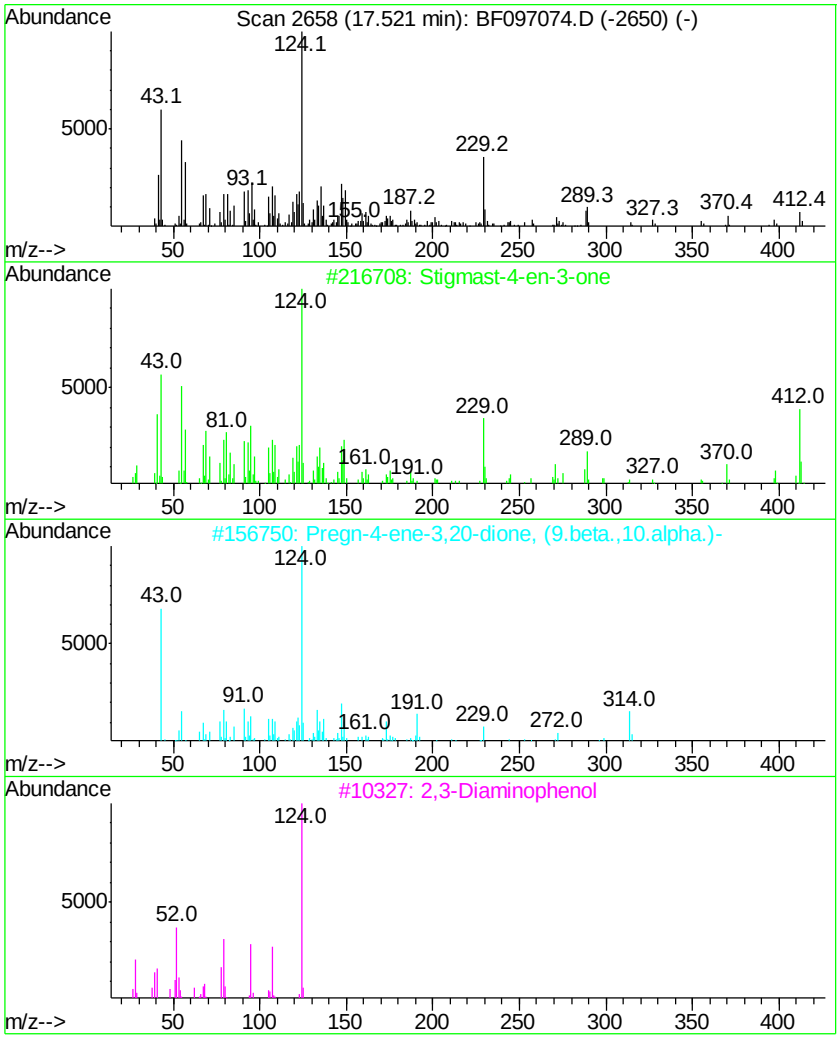
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

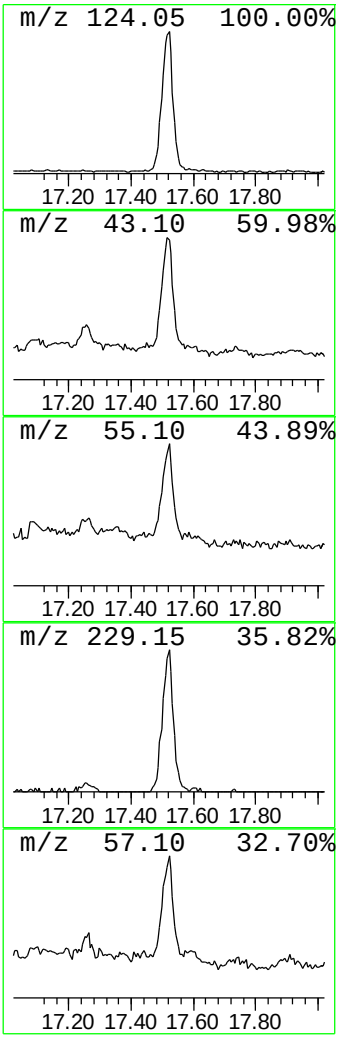
**********

Peak Number 20 Stigmast-4-en-3-one Concentration Rank 20

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.52 | 39.67 ng | 1069270 | Perylene-d12 | 14.98 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Stigmast-4-en-3-one | 412 | C29H48O | 001058-61-3 | 98 |
| 2 | Pregn-4-ene-3,20-dione, (9.beta.... | 314 | C21H30O2 | 002755-10-4 | 50 |
| 3 | 2,3-Diaminophenol | 124 | C6H8N2O | 059649-56-8 | 47 |
| 4 | 4,6-Dimethyl-2-pyrimidone | 124 | C6H8N2O | 000108-79-2 | 43 |
| 5 | 2-Methyl-4,5-pyrimidinediamine | 124 | C5H8N4 | 015579-63-2 | 43 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097074.D
Acq On : 26 Jul 2017 14:40
Operator : SJ/JU
Sample : I4443-05 5X
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** E2-M7-ESW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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 |
| Phenol, 2-ethyl-5... | 7.96 | 59.1 | ng | 1932400 | 2 | 7.78 | 653586 | 20.0 |
| Phenol, 4-ethyl-3... | 8.04 | 95.9 | ng | 3133080 | 2 | 7.78 | 653586 | 20.0 |
| Phenol, 3-ethyl-5... | 8.17 | 176.6 | ng | 5770160 | 2 | 7.78 | 653586 | 20.0 |
| Phenol, 3,4,5-tri... | 8.24 | 63.0 | ng | 2059450 | 2 | 7.78 | 653586 | 20.0 |
| Phenol, 2,4,6-tri... | 8.26 | 67.7 | ng | 2211260 | 2 | 7.78 | 653586 | 20.0 |
| Phenol, 2-methyl-... | 8.37 | 46.0 | ng | 1504100 | 2 | 7.78 | 653586 | 20.0 |
| Tetradecanoic acid | 10.76 | 175.0 | ng | 7528430 | 4 | 11.00 | 860602 | 20.0 |
| cis-9-Hexadecenoi... | 11.53 | 55.8 | ng | 2399120 | 4 | 11.00 | 860602 | 20.0 |
| n-Hexadecanoic acid | 11.65 | 427.1 | ng | 18376900 | 4 | 11.00 | 860602 | 20.0 |
| 10,18-Bisnorabiet... | 12.26 | 43.0 | ng | 1851980 | 4 | 11.00 | 860602 | 20.0 |
| cis-13-Octadeceno... | 12.37 | 737.8 | ng | 29522600 | 5 | 13.63 | 800293 | 20.0 |
| Octadecanoic acid | 12.43 | 123.8 | ng | 4952970 | 5 | 13.63 | 800293 | 20.0 |
| 9,12-Octadecadien... | 12.49 | 53.5 | ng | 2142570 | 5 | 13.63 | 800293 | 20.0 |
| unknown13.07 | 13.07 | 198.4 | ng | 7938180 | 5 | 13.63 | 800293 | 20.0 |
| unknown13.15 | 13.15 | 92.6 | ng | 3705620 | 5 | 13.63 | 800293 | 20.0 |
| Vitamin E | 15.60 | 51.7 | ng | 1394080 | 6 | 14.98 | 539087 | 20.0 |
| .gamma.-Sitosterol | 16.69 | 106.8 | ng | 2879060 | 6 | 14.98 | 539087 | 20.0 |
| Stigmast-4-en-3-one | 17.52 | 39.7 | ng | 1069270 | 6 | 14.98 | 539087 | 20.0 |