LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117660.D
Acq On : 31 Oct 2019 16:11
Operator : JU
Sample : K5541-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 153-63-(0-2)

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

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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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 | 5.357 | 553 | 556 | 577 | rBV | 361855 | 648399 | 79.64% | 7.974% |
| 2 | 6.387 | 728 | 731 | 747 | rBV | 517344 | 779477 | 95.74% | 9.587% |
| 3 | 6.504 | 747 | 751 | 767 | rVB | 794485 | 814197 | 100.00% | 10.014% |
| 4 | 6.728 | 786 | 789 | 799 | rVB | 202980 | 188936 | 23.21% | 2.324% |
| 5 | 6.881 | 812 | 815 | 827 | rBV | 519771 | 494210 | 60.70% | 6.078% |
| 6 | 7.298 | 882 | 886 | 901 | rBV | 282375 | 438731 | 53.89% | 5.396% |
| 7 | 8.010 | 1004 | 1007 | 1035 | rBV | 142403 | 245715 | 30.18% | 3.022% |
| 8 | 9.081 | 1186 | 1189 | 1208 | rBV | 503594 | 583732 | 71.69% | 7.179% |
| 9 | 9.486 | 1255 | 1258 | 1273 | rBB | 53015 | 65254 | 8.01% | 0.803% |
| 10 | 9.763 | 1301 | 1305 | 1320 | rBV | 263744 | 293197 | 36.01% | 3.606% |
| 11 | 10.557 | 1437 | 1440 | 1456 | rBV | 348727 | 437629 | 53.75% | 5.382% |
| 12 | 11.251 | 1554 | 1558 | 1561 | rBV | 269985 | 273767 | 33.62% | 3.367% |
| 13 | 11.275 | 1561 | 1562 | 1568 | rVV | 83540 | 78973 | 9.70% | 0.971% |
| 14 | 11.339 | 1570 | 1573 | 1581 | rVB | 12151 | 17070 | 2.10% | 0.210% |
| 15 | 11.757 | 1642 | 1644 | 1645 | rBV | 11792 | 9642 | 1.18% | 0.119% |
| 16 | 11.775 | 1645 | 1647 | 1655 | rVB3 | 31263 | 50424 | 6.19% | 0.620% |
| 17 | 11.869 | 1660 | 1663 | 1666 | rBV | 21633 | 23057 | 2.83% | 0.284% |
| 18 | 12.304 | 1734 | 1737 | 1739 | rBV2 | 11383 | 9809 | 1.20% | 0.121% |
| 19 | 12.410 | 1749 | 1755 | 1761 | rVB4 | 6152 | 10442 | 1.28% | 0.128% |
| 20 | 12.469 | 1761 | 1765 | 1774 | rBV | 238978 | 258864 | 31.79% | 3.184% |
| 21 | 12.698 | 1796 | 1804 | 1811 | rBV | 222422 | 283398 | 34.81% | 3.485% |
| 22 | 12.751 | 1811 | 1813 | 1818 | rVB | 8759 | 9687 | 1.19% | 0.119% |
| 23 | 12.827 | 1822 | 1826 | 1832 | rBV | 590708 | 499332 | 61.33% | 6.141% |
| 24 | 12.916 | 1838 | 1841 | 1848 | rVB2 | 13377 | 20559 | 2.53% | 0.253% |
| 25 | 13.010 | 1852 | 1857 | 1858 | rBV3 | 7735 | 11284 | 1.39% | 0.139% |
| 26 | 13.027 | 1858 | 1860 | 1868 | rVB3 | 21387 | 31249 | 3.84% | 0.384% |
| 27 | 13.092 | 1868 | 1871 | 1875 | rBV | 15866 | 17839 | 2.19% | 0.219% |
| 28 | 13.133 | 1875 | 1878 | 1882 | rVV4 | 14053 | 19934 | 2.45% | 0.245% |
| 29 | 13.227 | 1891 | 1894 | 1897 | rBV | 10412 | 10010 | 1.23% | 0.123% |
| 30 | 13.257 | 1897 | 1899 | 1905 | rVV3 | 12570 | 14595 | 1.79% | 0.179% |
| 31 | 13.557 | 1946 | 1950 | 1955 | rVB3 | 7684 | 10114 | 1.24% | 0.124% |
| 32 | 13.669 | 1963 | 1969 | 1972 | rBV4 | 17789 | 25809 | 3.17% | 0.317% |
| 33 | 13.704 | 1972 | 1975 | 1976 | rVV | 12837 | 11588 | 1.42% | 0.143% |
| 34 | 13.727 | 1976 | 1979 | 1990 | rVB5 | 69802 | 133659 | 16.42% | 1.644% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117660.D
Acq On : 31 Oct 2019 16:11
Operator : JU
Sample : K5541-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 153-63-(0-2)

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

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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 13.898 | 2002 | 2008 | 2011 | rBV2 | 240453 | 340378 | 41.81% | 4.186% |
| 36 | 13.921 | 2011 | 2012 | 2020 | rVB | 84472 | 81298 | 9.99% | 1.000% |
| 37 | 14.004 | 2023 | 2026 | 2029 | rBV | 18295 | 15058 | 1.85% | 0.185% |
| 38 | 14.145 | 2048 | 2050 | 2057 | rVB6 | 5432 | 8448 | 1.04% | 0.104% |
| 39 | 14.292 | 2070 | 2075 | 2079 | rBV2 | 17279 | 22638 | 2.78% | 0.278% |
| 40 | 14.339 | 2079 | 2083 | 2085 | rVV3 | 13341 | 15389 | 1.89% | 0.189% |
| 41 | 14.368 | 2085 | 2088 | 2094 | rVB6 | 16322 | 27728 | 3.41% | 0.341% |
| 42 | 14.639 | 2130 | 2134 | 2137 | rVB3 | 18602 | 19869 | 2.44% | 0.244% |
| 43 | 14.704 | 2142 | 2145 | 2149 | rVB | 13204 | 13140 | 1.61% | 0.162% |
| 44 | 14.927 | 2179 | 2183 | 2186 | rBV | 81357 | 115535 | 14.19% | 1.421% |
| 45 | 14.951 | 2186 | 2187 | 2193 | rVB2 | 60193 | 57599 | 7.07% | 0.708% |
| 46 | 15.033 | 2198 | 2201 | 2205 | rVB | 18708 | 24544 | 3.01% | 0.302% |
| 47 | 15.215 | 2228 | 2232 | 2239 | rVB | 45812 | 51821 | 6.36% | 0.637% |
| 48 | 15.280 | 2239 | 2243 | 2249 | rBV | 68300 | 102395 | 12.58% | 1.259% |
| 49 | 15.333 | 2249 | 2252 | 2264 | rVB2 | 135563 | 204462 | 25.11% | 2.515% |
| 50 | 15.710 | 2311 | 2316 | 2320 | rVB2 | 23767 | 33672 | 4.14% | 0.414% |
| 51 | 15.786 | 2322 | 2329 | 2331 | rBV3 | 10048 | 18342 | 2.25% | 0.226% |
| 52 | 16.174 | 2390 | 2395 | 2399 | rBV4 | 11730 | 19540 | 2.40% | 0.240% |
| 53 | 16.574 | 2458 | 2463 | 2466 | rBV5 | 6342 | 9985 | 1.23% | 0.123% |
| 54 | 16.727 | 2481 | 2489 | 2491 | rBV6 | 6731 | 16420 | 2.02% | 0.202% |
| 55 | 16.768 | 2491 | 2496 | 2504 | rVB3 | 26278 | 54097 | 6.64% | 0.665% |
| 56 | 17.198 | 2564 | 2569 | 2579 | rBV2 | 21379 | 48005 | 5.90% | 0.590% |
| 57 | 17.462 | 2608 | 2614 | 2616 | rBV5 | 7258 | 10024 | 1.23% | 0.123% |

Sum of corrected areas: 8130969

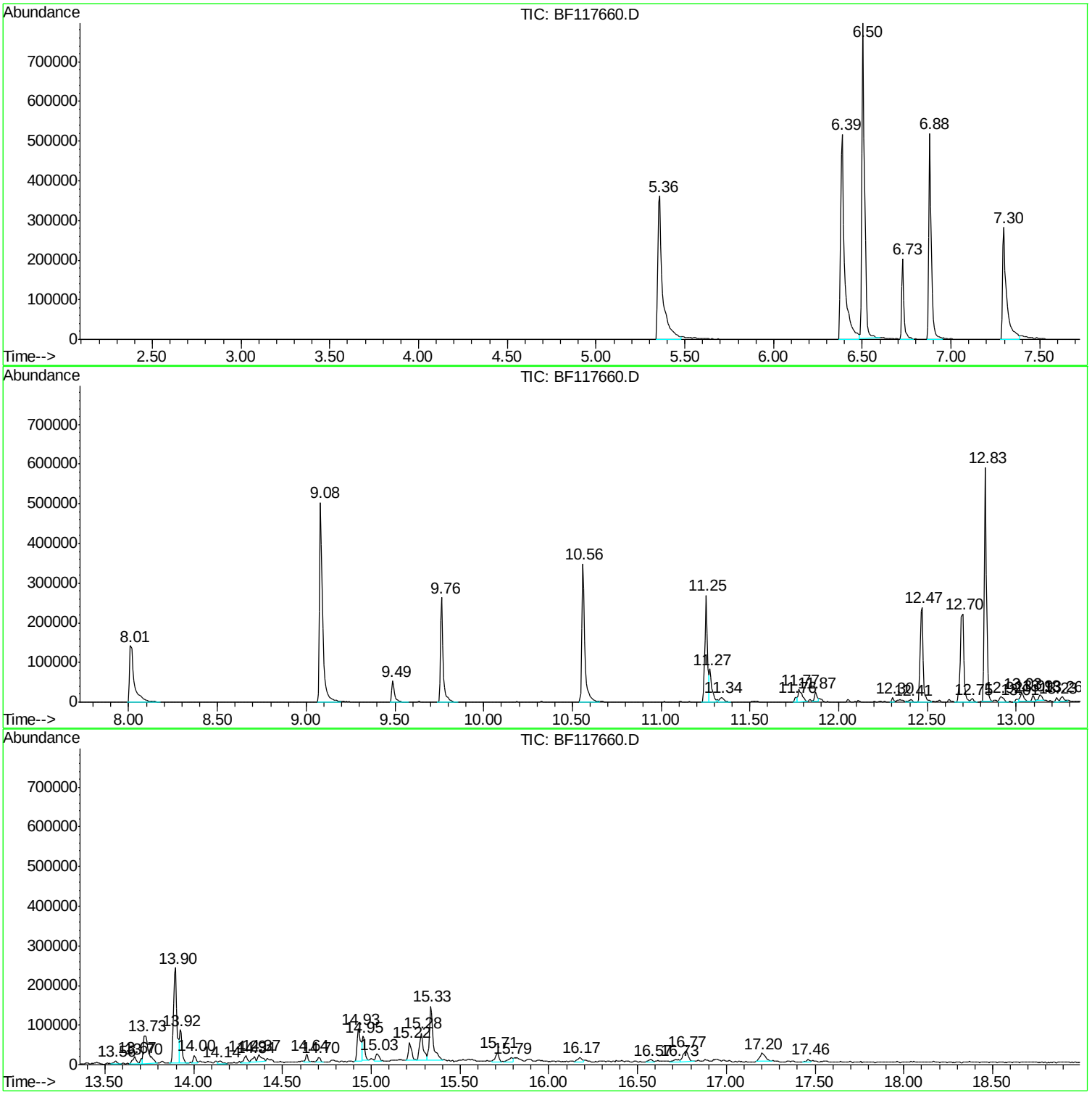
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117660.D
Acq On : 31 Oct 2019 16:11
Operator : JU
Sample : K5541-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 153-63-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117660.D
Acq On : 31 Oct 2019 16:11
Operator : JU
Sample : K5541-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 153-63-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

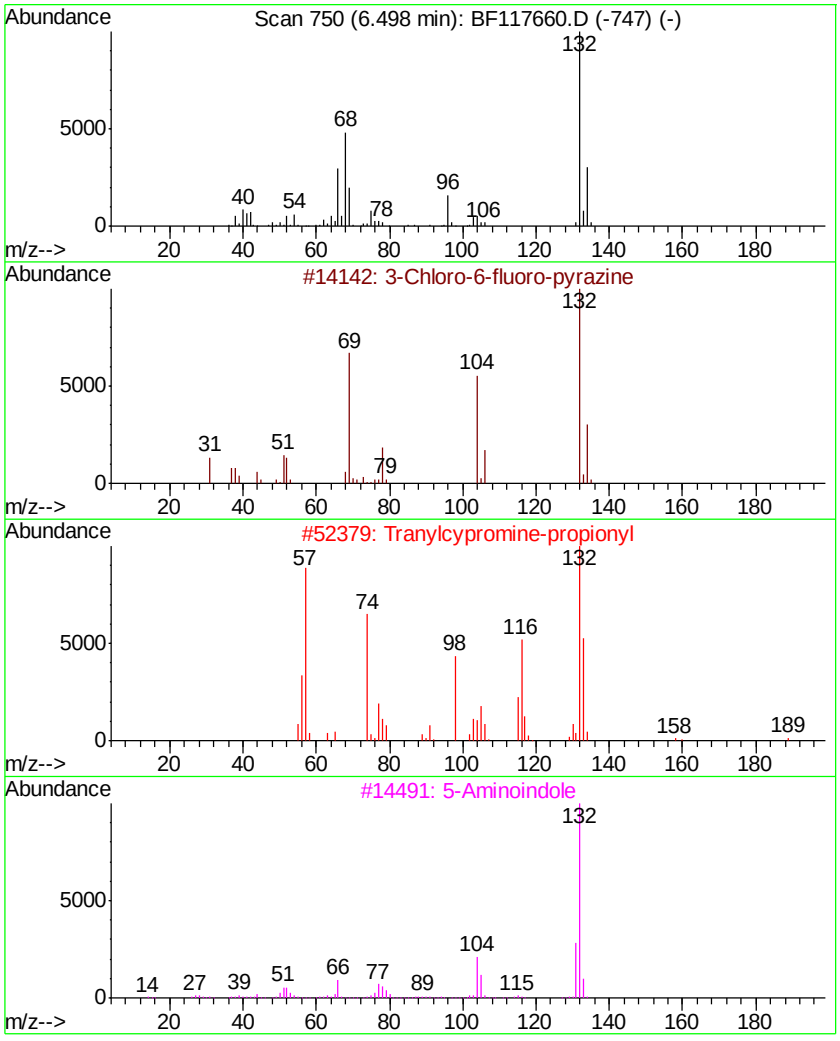
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

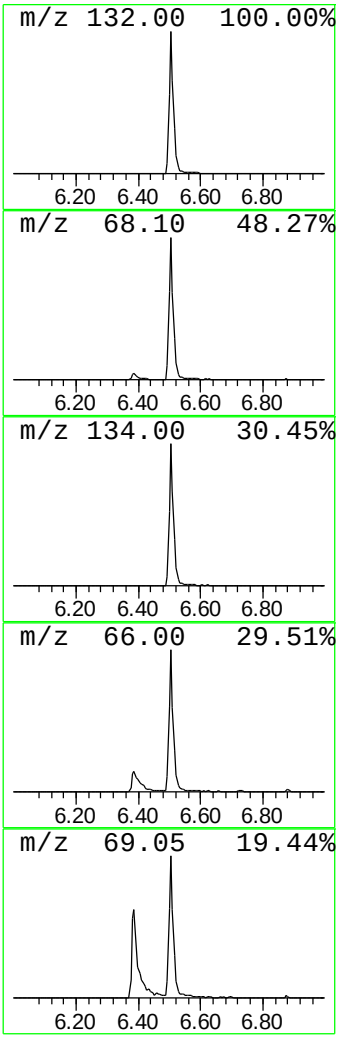
**********

Peak Number 1 unknown6.50 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.50 | 86.19 ng | 814197 | 1,4-Dichlorobenzene-d4 | 6.73 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 16 |
| 2 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 3 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 4 | 1,2,4-Trifluorobenzene | 132 | C6H3F3 | 000367-23-7 | 9 |
| 5 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117660.D
Acq On : 31 Oct 2019 16:11
Operator : JU
Sample : K5541-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 153-63-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

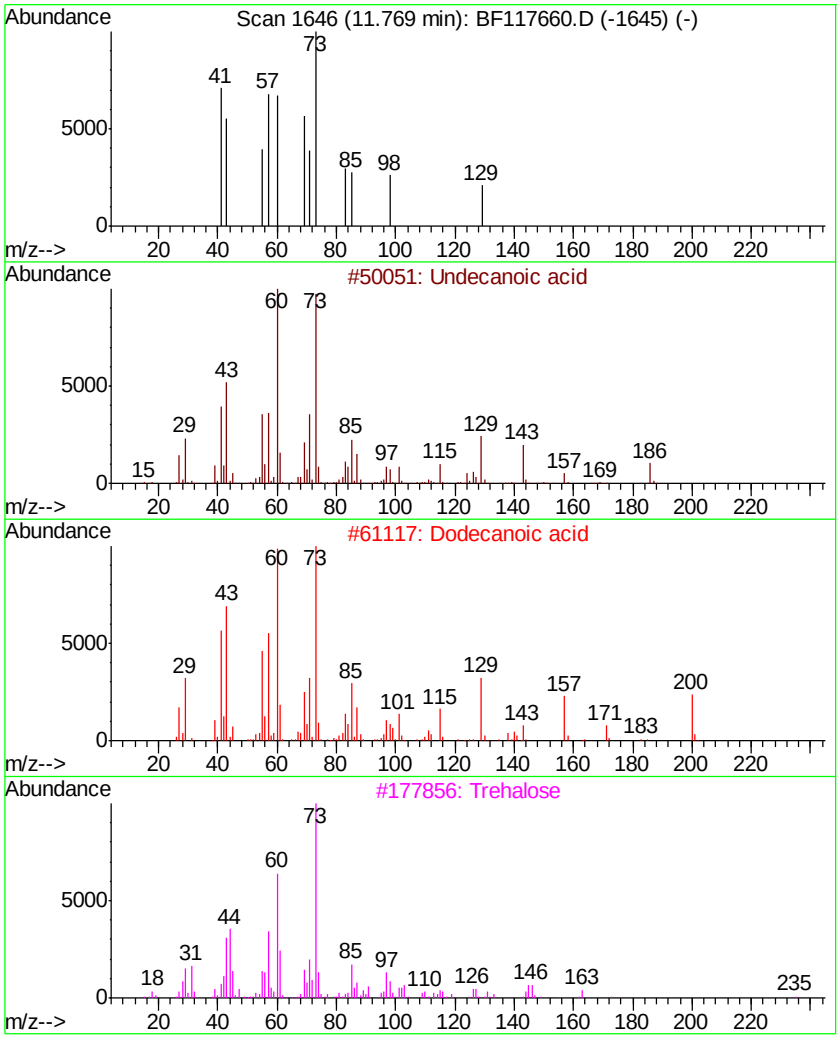
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

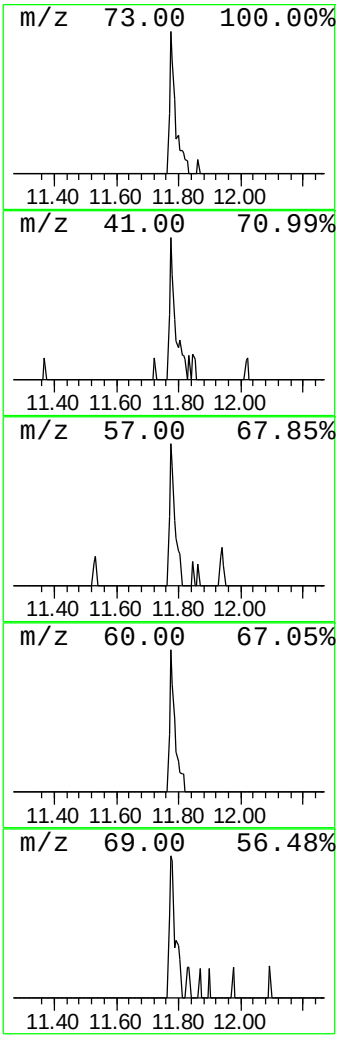
**********

Peak Number 3 Undecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.77 | 3.68 ng | 50424 | Phenanthrene-d10 | 11.25 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 50 |
| 2 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 50 |
| 3 | Trehalose | 342 | C12H22O11 | 000099-20-7 | 47 |
| 4 | Lactose | 342 | C12H22O11 | 000063-42-3 | 43 |
| 5 | n-Decanoic acid | 172 | C10H20O2 | 000334-48-5 | 38 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117660.D
Acq On : 31 Oct 2019 16:11
Operator : JU
Sample : K5541-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 153-63-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

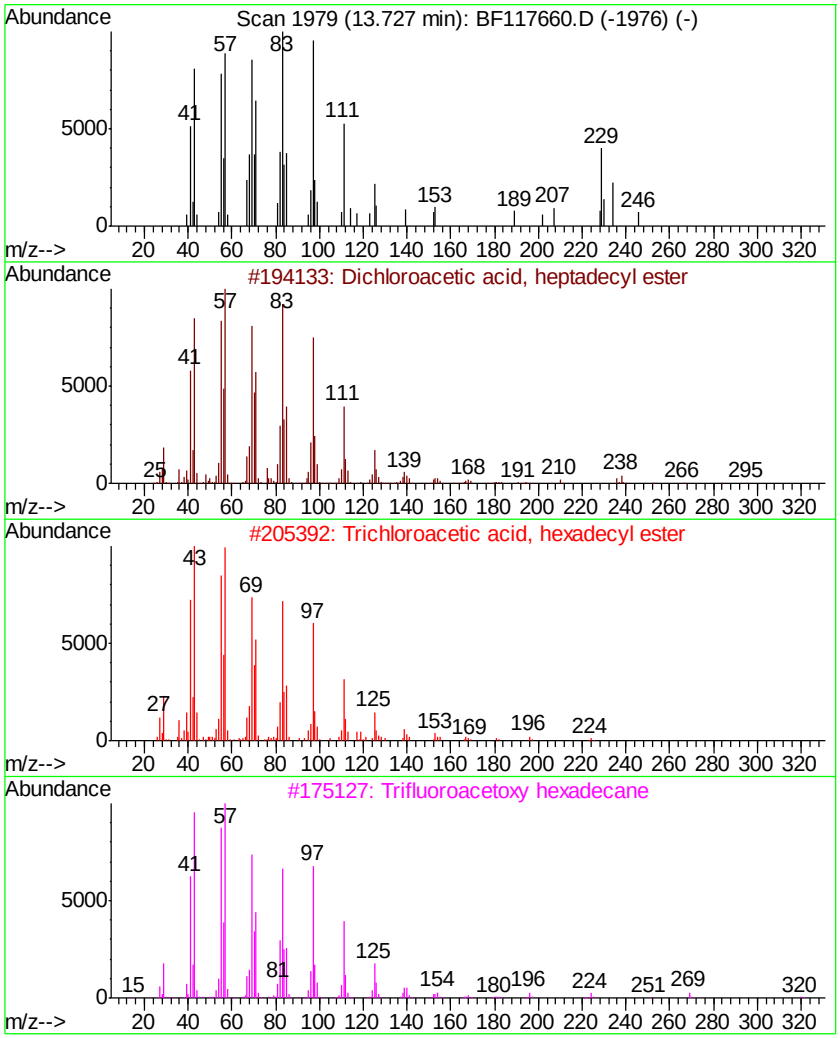
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

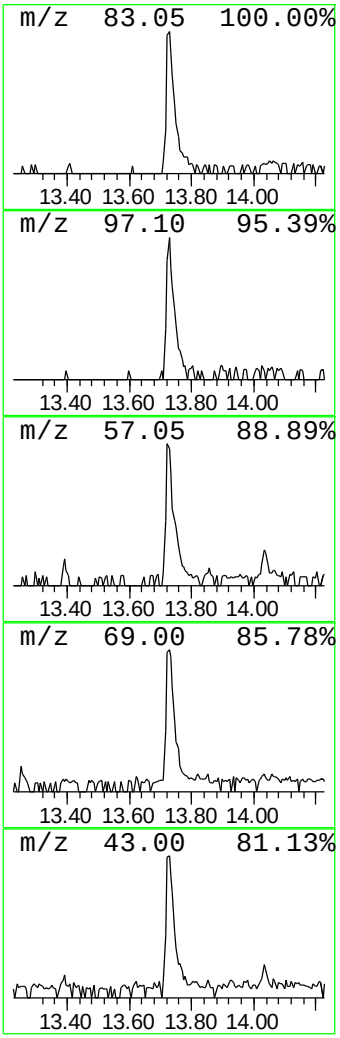
**********

Peak Number 4 Dichloroacetic acid, heptad... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.73 | 7.85 ng | 133659 | Chrysene-d12 | 13.90 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Dichloroacetic acid, heptadecyl ... | 366 | C19H36Cl2O2 | 1000282-98-2 | 81 |
| 2 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 81 |
| 3 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 81 |
| 4 | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1 | 81 |
| 5 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 81 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117660.D
Acq On : 31 Oct 2019 16:11
Operator : JU
Sample : K5541-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 153-63-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

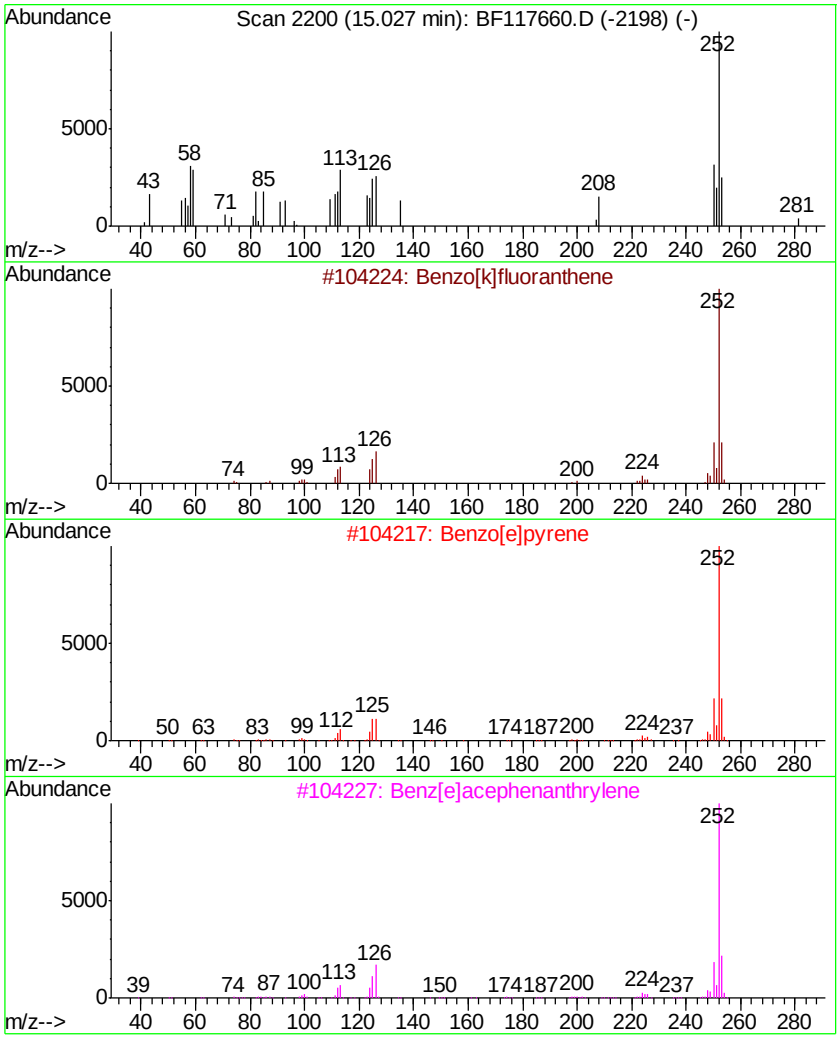
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

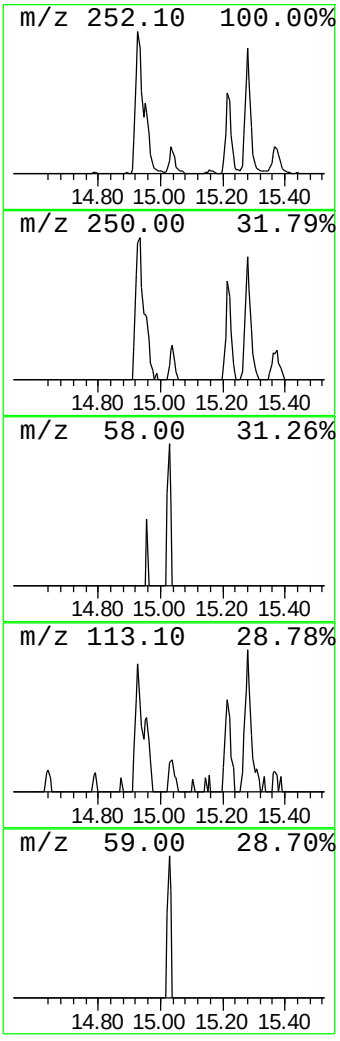
**********

Peak Number 5 Benzo[e]pyrene Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.03 | 2.40 ng | 24544 | Perylene-d12 | 15.33 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzo[k]fluoranthene | 252 | C20H12 | 000207-08-9 | 87 |
| 2 | Benzo[e]pyrene | 252 | C20H12 | 000192-97-2 | 80 |
| 3 | Benz[e]acephenanthrylene | 252 | C20H12 | 000205-99-2 | 80 |
| 4 | Perylene | 252 | C20H12 | 000198-55-0 | 74 |
| 5 | Benzo[a]pyrene | 252 | C20H12 | 000050-32-8 | 74 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117660.D
Acq On : 31 Oct 2019 16:11
Operator : JU
Sample : K5541-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 153-63-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

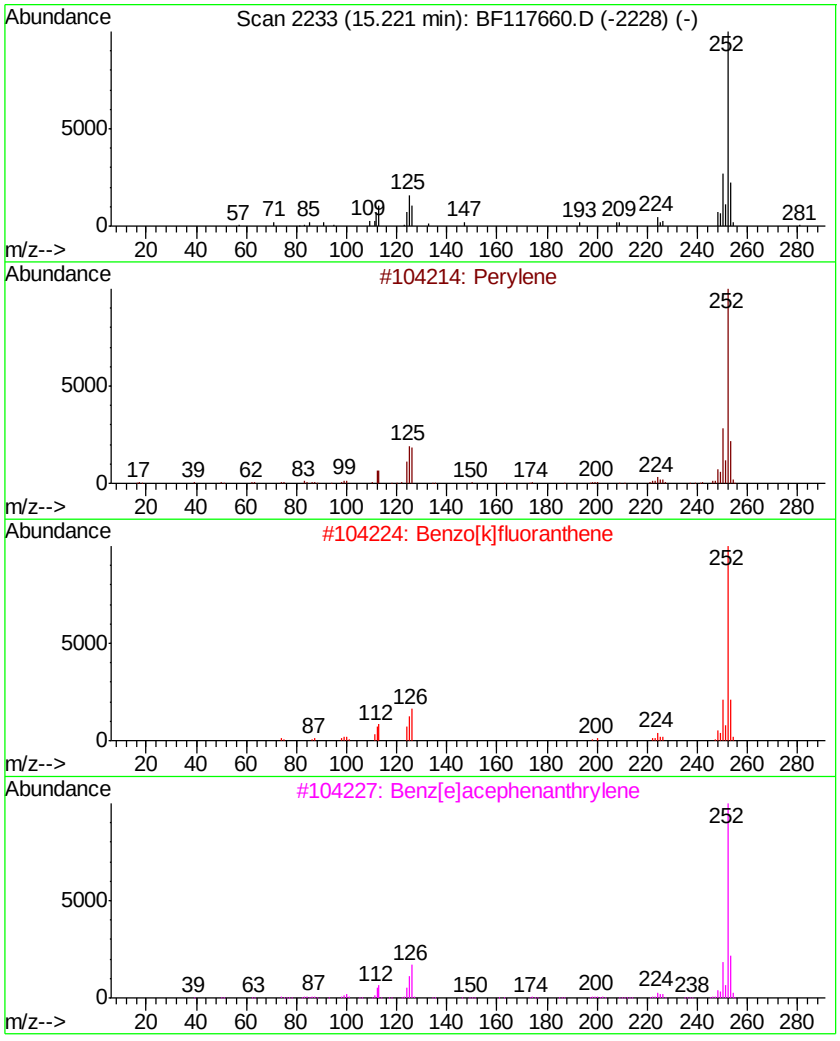
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

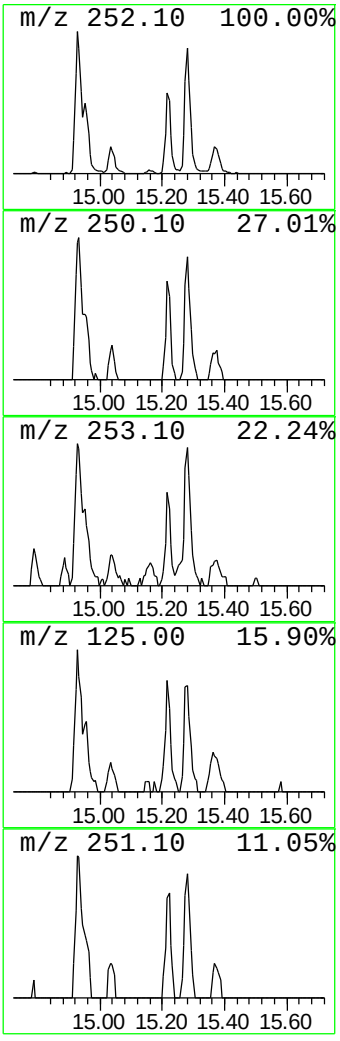
**********

Peak Number 6 Perylene Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.22 | 5.07 ng | 51821 | Perylene-d12 | 15.33 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Perylene | 252 | C20H12 | 000198-55-0 | 98 |
| 2 | Benzo[k]fluoranthene | 252 | C20H12 | 000207-08-9 | 97 |
| 3 | Benz[e]acephenanthrylene | 252 | C20H12 | 000205-99-2 | 96 |
| 4 | Benzo[e]pyrene | 252 | C20H12 | 000192-97-2 | 96 |
| 5 | Benzo[j]fluoranthene | 252 | C20H12 | 000205-82-3 | 94 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117660.D
Acq On : 31 Oct 2019 16:11
Operator : JU
Sample : K5541-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 153-63-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

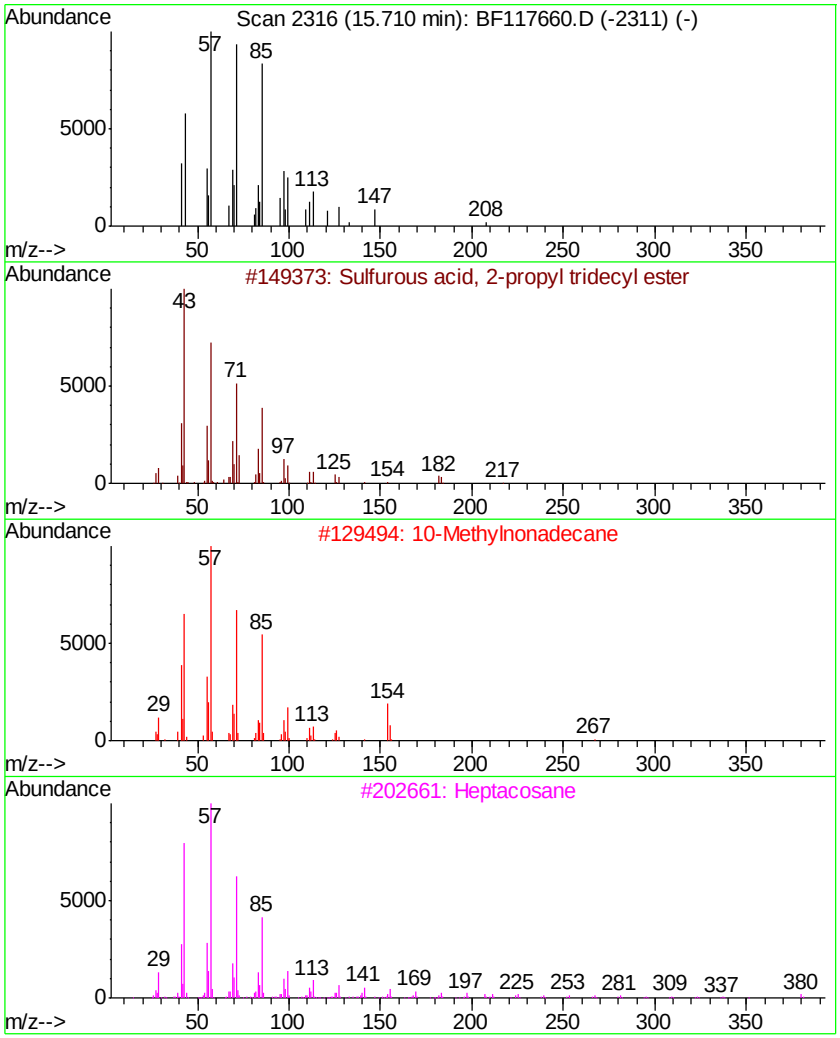
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

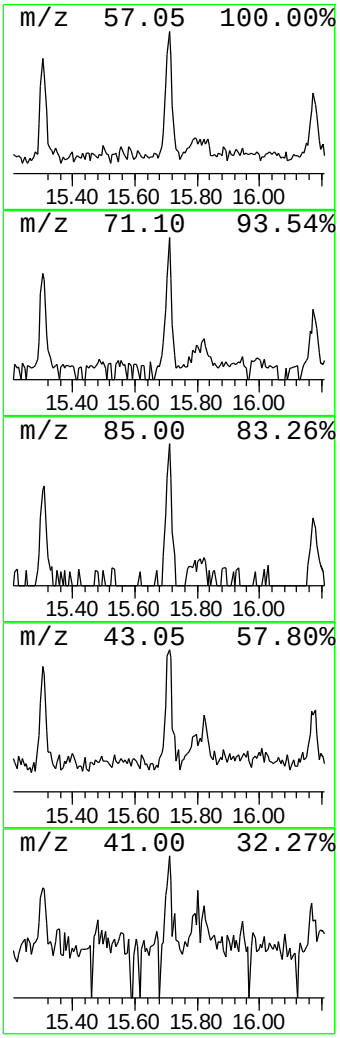
**********

Peak Number 7 Sulfurous acid, 2-propyl tr... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.71 | 3.29 ng | 33672 | Perylene-d12 | 15.33 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Sulfurous acid, 2-propyl tridecy... | 306 | C16H34O3S | 1000309-12-4 | 83 |
| 2 | 10-Methylnonadecane | 282 | C20H42 | 056862-62-5 | 80 |
| 3 | Heptacosane | 380 | C27H56 | 000593-49-7 | 78 |
| 4 | Hexatriacontane | 507 | C36H74 | 000630-06-8 | 78 |
| 5 | Sulfurous acid, 2-propyl tetrade... | 320 | C17H36O3S | 1000309-12-5 | 72 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF103119\
Data File : BF117660.D
Acq On : 31 Oct 2019 16:11
Operator : JU
Sample : K5541-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** 153-63-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| unknown6.50 | 6.50 | 86.2 | ng | 814197 | 1 | 6.73 | 188936 | 20.0 |
| Undecanoic acid | 11.77 | 3.7 | ng | 50424 | 4 | 11.25 | 273767 | 20.0 |
| Dichloroacetic ac... | 13.73 | 7.8 | ng | 133659 | 5 | 13.90 | 340378 | 20.0 |
| Benzo[e]pyrene | 15.03 | 2.4 | ng | 24544 | 6 | 15.33 | 204462 | 20.0 |
| Perylene | 15.22 | 5.1 | ng | 51821 | 6 | 15.33 | 204462 | 20.0 |
| Sulfurous acid, 2... | 15.71 | 3.3 | ng | 33672 | 6 | 15.33 | 204462 | 20.0 |