LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091317\
Data File : BF098507.D
Acq On : 13 Sep 2017 23:32
Operator : SJ/JU
Sample : I5160-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** G-7-1

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-BF091117.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 | 4.851 | 467 | 470 | 486 | rBV | 244228 | 413670 | 8.10% | 0.953% |
| 2 | 5.275 | 537 | 542 | 557 | rBV | 4752310 | 4944859 | 96.84% | 11.391% |
| 3 | 6.316 | 714 | 719 | 734 | rBV | 4420250 | 5106026 | 100.00% | 11.763% |
| 4 | 6.434 | 734 | 739 | 742 | rBV | 4923052 | 4678711 | 91.63% | 10.778% |
| 5 | 6.657 | 773 | 777 | 784 | rVB | 1205776 | 1043295 | 20.43% | 2.403% |
| 6 | 6.810 | 799 | 803 | 807 | rBV | 3597606 | 3462669 | 67.82% | 7.977% |
| 7 | 7.228 | 869 | 874 | 877 | rBV | 2882576 | 2717079 | 53.21% | 6.259% |
| 8 | 7.939 | 991 | 995 | 998 | rBV | 1600483 | 1342311 | 26.29% | 3.092% |
| 9 | 8.498 | 1086 | 1090 | 1094 | rBV | 278017 | 250782 | 4.91% | 0.578% |
| 10 | 9.016 | 1172 | 1178 | 1181 | rBV | 4620330 | 4153392 | 81.34% | 9.568% |
| 11 | 9.410 | 1241 | 1245 | 1252 | rVB | 703944 | 591173 | 11.58% | 1.362% |
| 12 | 9.551 | 1265 | 1269 | 1272 | rBV | 72952 | 62208 | 1.22% | 0.143% |
| 13 | 9.686 | 1284 | 1292 | 1296 | rBV | 1449049 | 1327171 | 25.99% | 3.057% |
| 14 | 10.404 | 1409 | 1414 | 1417 | rBV | 797568 | 750289 | 14.69% | 1.728% |
| 15 | 10.480 | 1422 | 1427 | 1430 | rBV | 2001064 | 1905264 | 37.31% | 4.389% |
| 16 | 10.604 | 1443 | 1448 | 1454 | rVB4 | 42571 | 63027 | 1.23% | 0.145% |
| 17 | 11.169 | 1540 | 1544 | 1546 | rBV | 1286291 | 1068148 | 20.92% | 2.461% |
| 18 | 11.192 | 1546 | 1548 | 1551 | rVV | 438028 | 333882 | 6.54% | 0.769% |
| 19 | 11.245 | 1551 | 1557 | 1560 | rVB | 161987 | 154555 | 3.03% | 0.356% |
| 20 | 11.404 | 1579 | 1584 | 1592 | rBV2 | 41888 | 69252 | 1.36% | 0.160% |
| 21 | 11.669 | 1625 | 1629 | 1632 | rBV | 58035 | 58426 | 1.14% | 0.135% |
| 22 | 11.698 | 1632 | 1634 | 1639 | rVB | 75350 | 63988 | 1.25% | 0.147% |
| 23 | 11.780 | 1645 | 1648 | 1650 | rBV | 94199 | 87925 | 1.72% | 0.203% |
| 24 | 12.110 | 1699 | 1704 | 1708 | rBV3 | 70159 | 76243 | 1.49% | 0.176% |
| 25 | 12.216 | 1719 | 1722 | 1726 | rBV | 53232 | 59757 | 1.17% | 0.138% |
| 26 | 12.257 | 1726 | 1729 | 1734 | rVB5 | 46904 | 67626 | 1.32% | 0.156% |
| 27 | 12.380 | 1746 | 1750 | 1754 | rBV | 559039 | 519994 | 10.18% | 1.198% |
| 28 | 12.604 | 1781 | 1788 | 1791 | rBV | 563057 | 613029 | 12.01% | 1.412% |
| 29 | 12.657 | 1794 | 1797 | 1802 | rVB3 | 45169 | 61175 | 1.20% | 0.141% |
| 30 | 12.751 | 1809 | 1813 | 1820 | rVB | 2830951 | 2695068 | 52.78% | 6.209% |
| 31 | 12.827 | 1822 | 1826 | 1830 | rBV3 | 41625 | 66492 | 1.30% | 0.153% |
| 32 | 12.933 | 1837 | 1844 | 1847 | rBV2 | 72399 | 125012 | 2.45% | 0.288% |
| 33 | 13.039 | 1858 | 1862 | 1864 | rBV | 74586 | 84140 | 1.65% | 0.194% |
| 34 | 13.239 | 1893 | 1896 | 1901 | rVB3 | 72183 | 89156 | 1.75% | 0.205% |

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091317\
Data File : BF098507.D
Acq On : 13 Sep 2017 23:32
Operator : SJ/JU
Sample : I5160-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** G-7-1

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-BF091117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 13.445 | 1928 | 1931 | 1938 | rVB | 73494 | 80247 | 1.57% | 0.185% |
| 36 | 13.651 | 1963 | 1966 | 1970 | rBV2 | 278379 | 289467 | 5.67% | 0.667% |
| 37 | 13.804 | 1987 | 1992 | 1994 | rBV2 | 1212915 | 1316826 | 25.79% | 3.034% |
| 38 | 13.827 | 1994 | 1996 | 2004 | rVB | 329869 | 302533 | 5.93% | 0.697% |
| 39 | 13.904 | 2005 | 2009 | 2011 | rBV3 | 89994 | 97513 | 1.91% | 0.225% |
| 40 | 14.192 | 2055 | 2058 | 2061 | rVB | 96433 | 88200 | 1.73% | 0.203% |
| 41 | 14.268 | 2067 | 2071 | 2072 | rBV3 | 54768 | 74578 | 1.46% | 0.172% |
| 42 | 14.604 | 2126 | 2128 | 2131 | rVB4 | 61995 | 54470 | 1.07% | 0.125% |
| 43 | 14.810 | 2159 | 2163 | 2166 | rBV | 341547 | 470069 | 9.21% | 1.083% |
| 44 | 15.086 | 2207 | 2210 | 2216 | rVB | 198019 | 229660 | 4.50% | 0.529% |
| 45 | 15.145 | 2216 | 2220 | 2225 | rBV | 245659 | 279595 | 5.48% | 0.644% |
| 46 | 15.204 | 2225 | 2230 | 2237 | rVV | 723075 | 892461 | 17.48% | 2.056% |
| 47 | 16.533 | 2453 | 2456 | 2464 | rBV3 | 74167 | 127199 | 2.49% | 0.293% |

Sum of corrected areas: 43408612

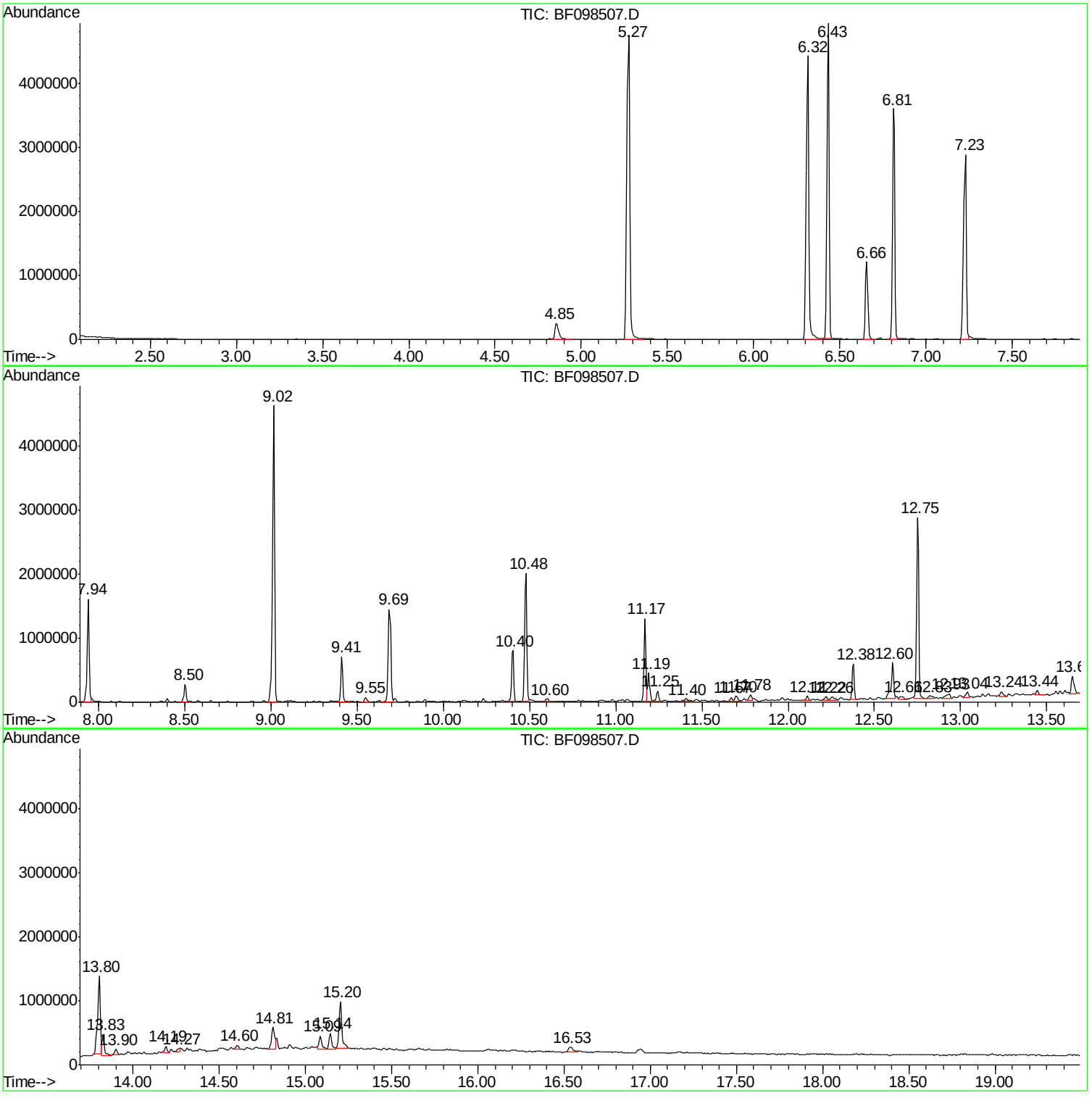
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091317\
Data File : BF098507.D
Acq On : 13 Sep 2017 23:32
Operator : SJ/JU
Sample : I5160-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** G-7-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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 : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091317\
Data File : BF098507.D
Acq On : 13 Sep 2017 23:32
Operator : SJ/JU
Sample : I5160-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** G-7-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

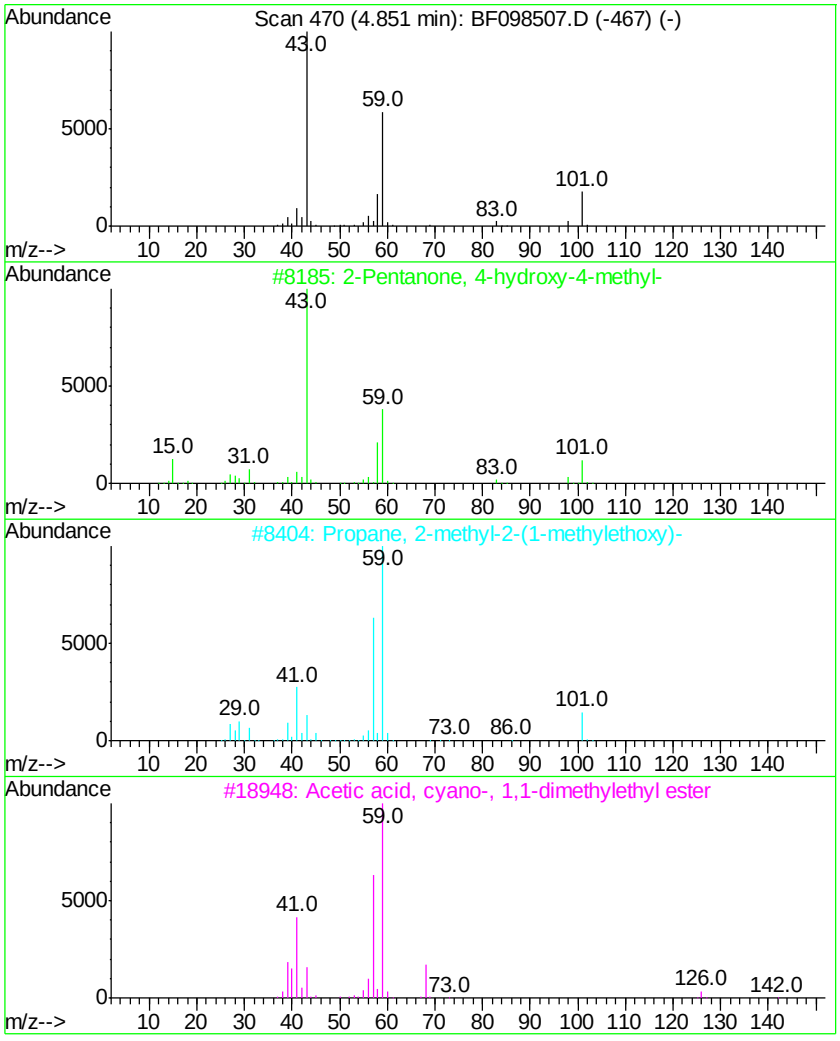
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

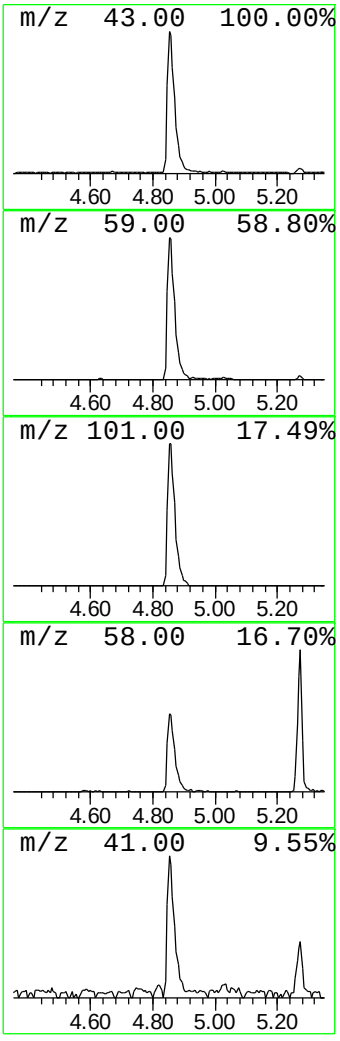
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.85 | 7.93 ng | 413670 | 1,4-Dichlorobenzene-d4 | 6.66 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 59 |
| 2 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 42 |
| 3 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23 |
| 4 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 10 |
| 5 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |



Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091317\
Data File : BF098507.D
Acq On : 13 Sep 2017 23:32
Operator : SJ/JU
Sample : I5160-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** G-7-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

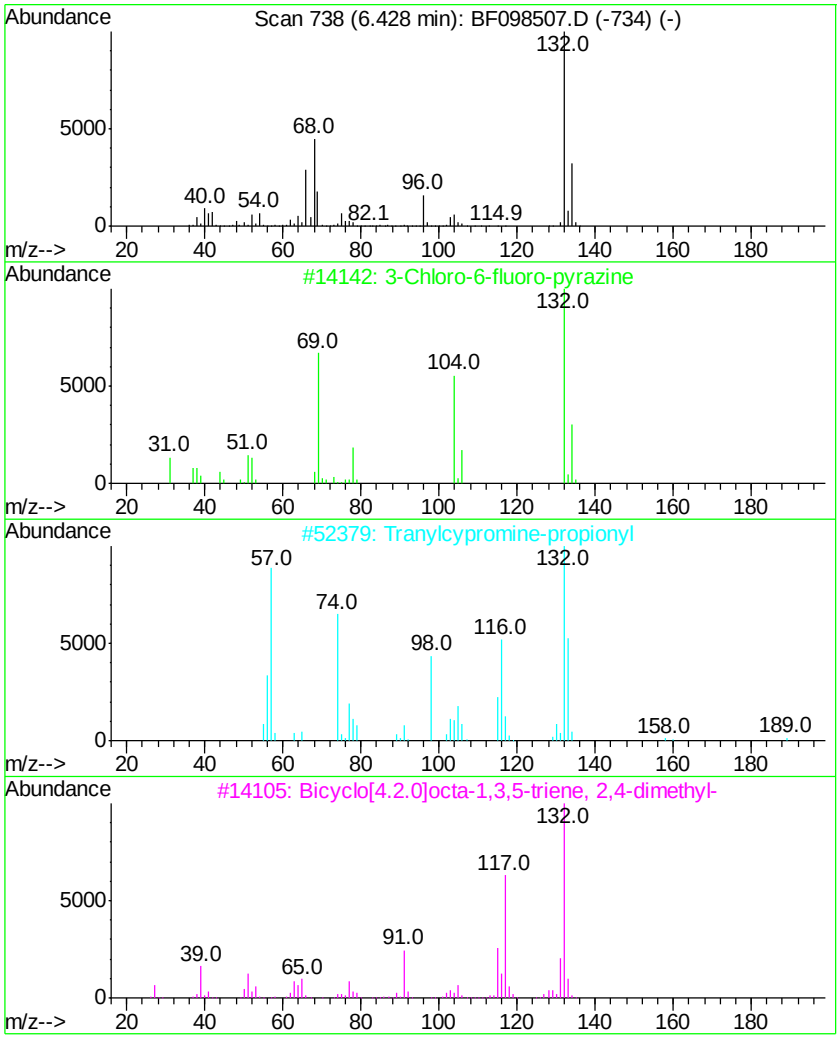
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

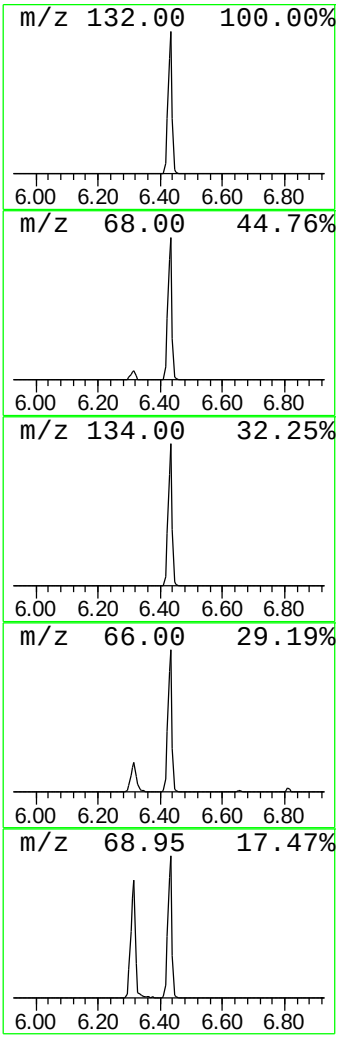
**********

Peak Number 2 unknown6.43 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.43 | 89.69 ng | 4678710 | 1,4-Dichlorobenzene-d4 | 6.66 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 3 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 4 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |
| 5 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |



# Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091317\
Data File : BF098507.D
Acq On : 13 Sep 2017 23:32
Operator : SJ/JU
Sample : I5160-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** G-7-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

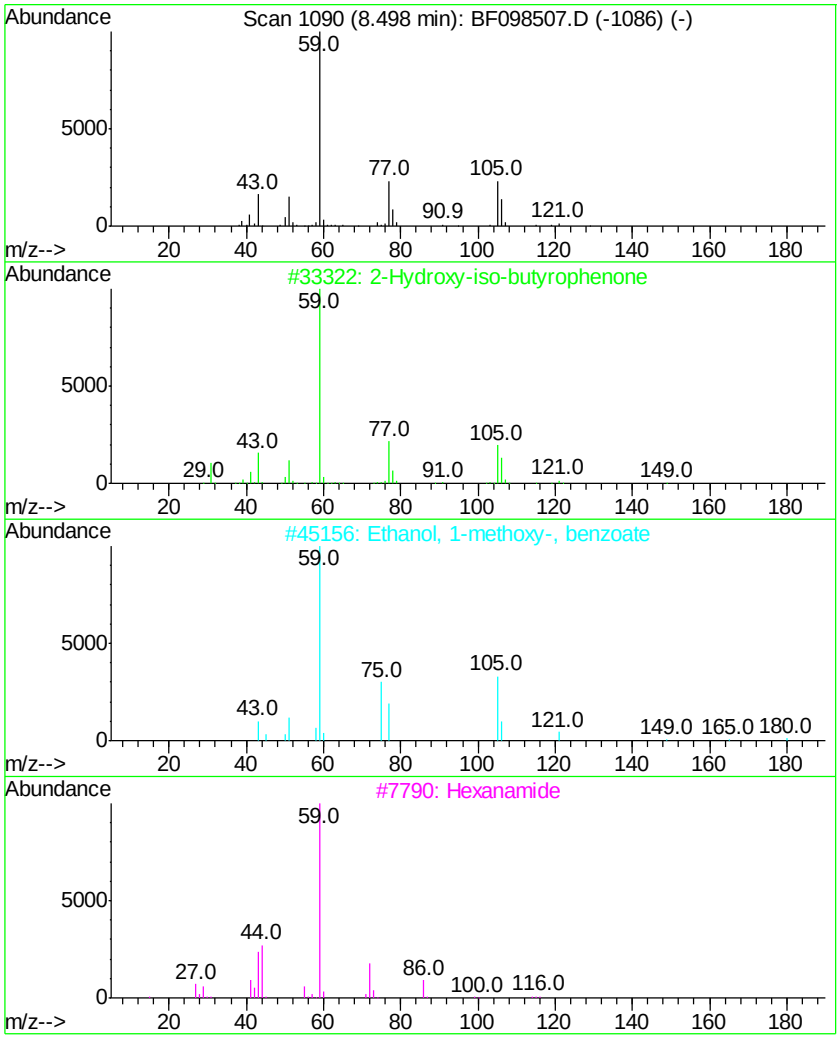
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

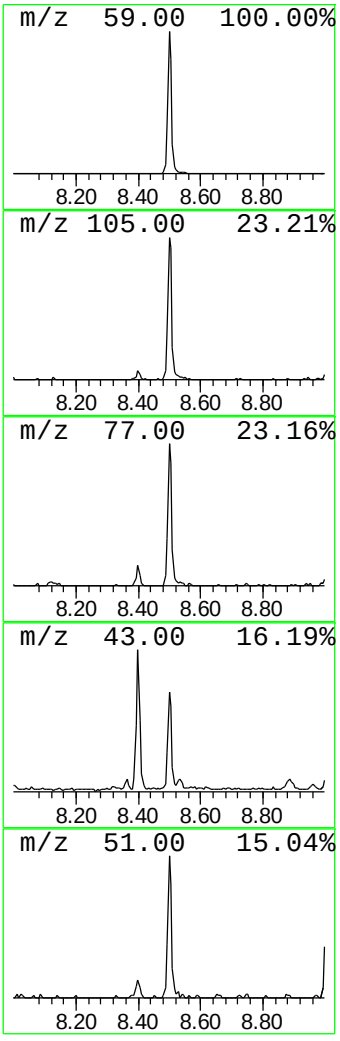
**********

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.50 | 3.74 ng | 250782 | Naphthalene-d8 | 7.94 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Hydroxy-iso-butyrophenone | 164 | C10H12O2 | 007473-98-5 | 90 |
| 2 | Ethanol, 1-methoxy-, benzoate | 180 | C10H12O3 | 051835-44-0 | 72 |
| 3 | Hexanamide | 115 | C6H13NO | 000628-02-4 | 9 |
| 4 | Propanoic acid, 2-hydroxy-2-meth... | 132 | C6H12O3 | 000080-55-7 | 9 |
| 5 | Guanidine | 59 | CH5N3 | 000113-00-8 | 7 |



Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091317\
Data File : BF098507.D
Acq On : 13 Sep 2017 23:32
Operator : SJ/JU
Sample : I5160-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** G-7-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

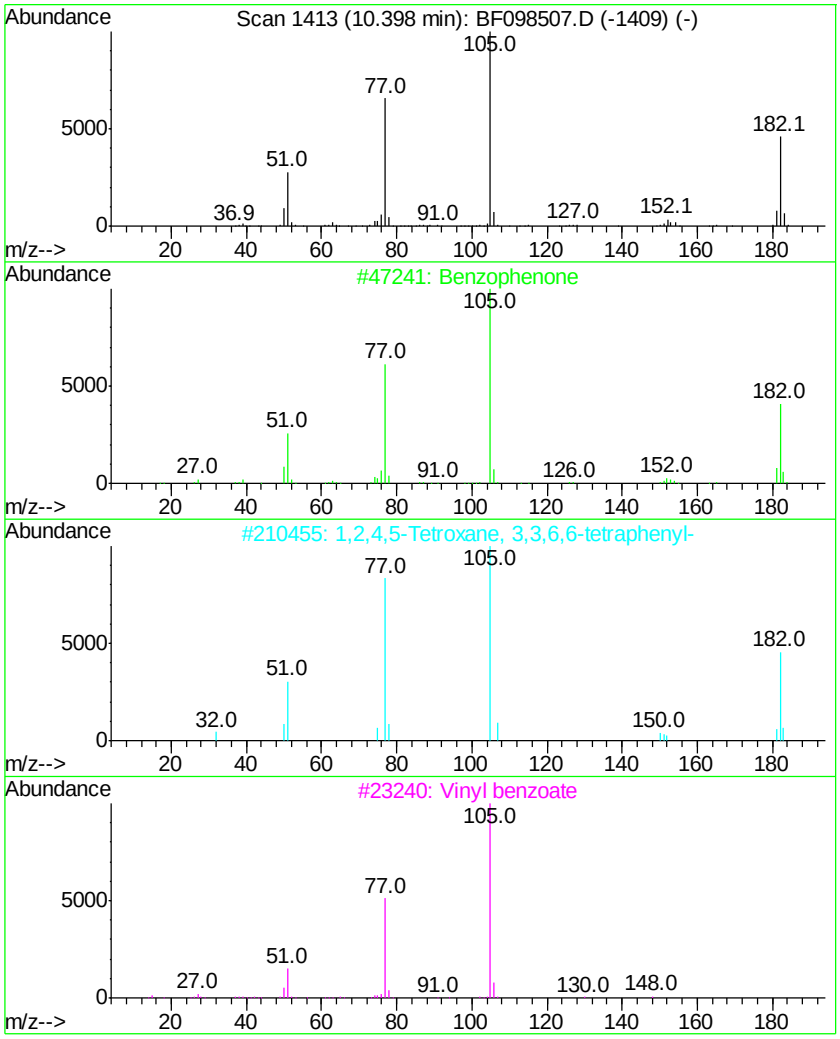
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

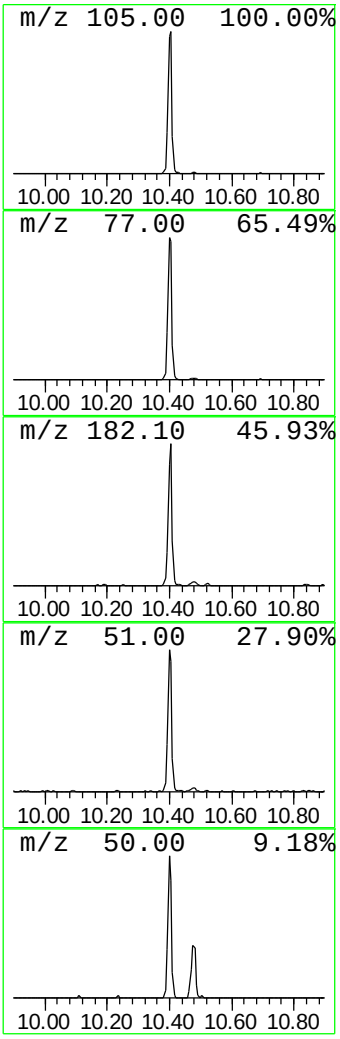
**********

Peak Number 5 Benzophenone Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.40 | 11.31 ng | 750289 | Acenaphthene-d10 | 9.69 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzophenone | 182 | C13H10O | 000119-61-9 | 97 |
| 2 | 1,2,4,5-Tetroxane, 3,3,6,6-tetra... | 396 | C26H20O4 | 016204-36-7 | 78 |
| 3 | Vinyl benzoate | 148 | C9H8O2 | 000769-78-8 | 47 |
| 4 | Benzenebutanoic acid, .gamma.-oxo- | 178 | C10H10O3 | 002051-95-8 | 47 |
| 5 | 1-Propanone, 2-bromo-1-phenyl- | 212 | C9H9BrO | 002114-00-3 | 47 |



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091317\
Data File : BF098507.D
Acq On : 13 Sep 2017 23:32
Operator : SJ/JU
Sample : I5160-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** G-7-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

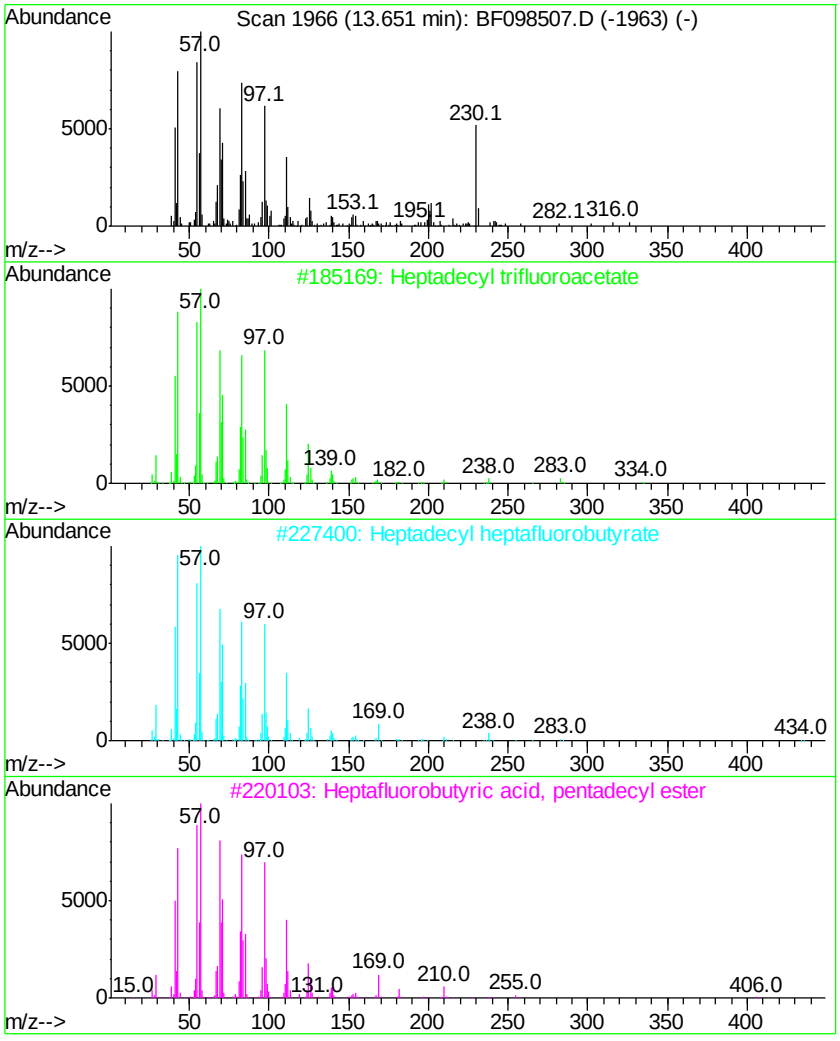
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

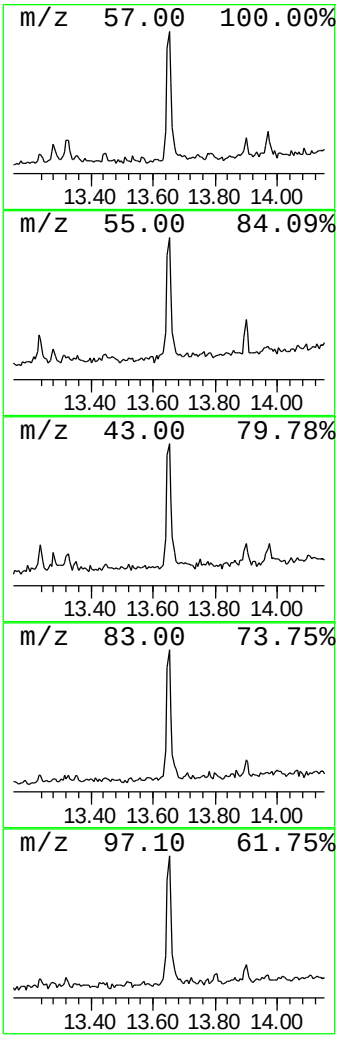
**********

Peak Number 6 Heptadecyl trifluoroacetate Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.65 | 4.40 ng | 289467 | Chrysene-d12 | 13.80 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecyl trifluoroacetate | 352 | C19H35F3O2 | 1000351-87-0 | 91 |
| 2 | Heptadecyl heptafluorobutyrate | 452 | C21H35F7O2 | 959085-66-6 | 90 |
| 3 | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 90 |
| 4 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 90 |
| 5 | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1 | 90 |



# Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091317\
Data File : BF098507.D
Acq On : 13 Sep 2017 23:32
Operator : SJ/JU
Sample : I5160-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** G-7-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

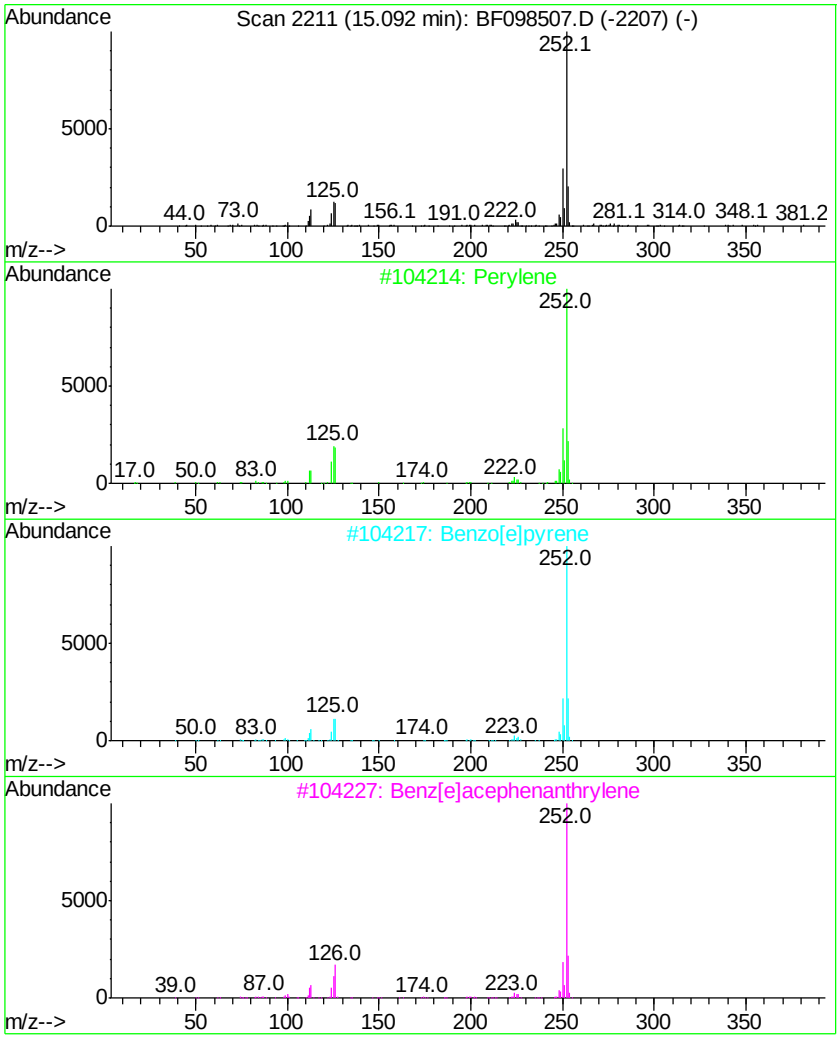
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

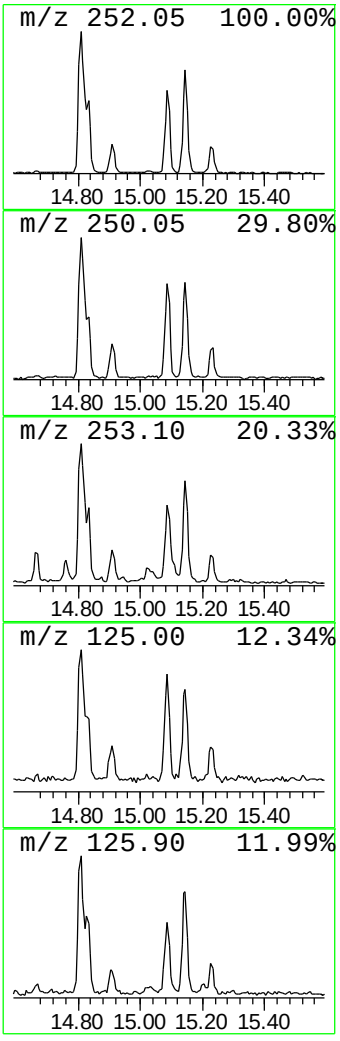
**********

Peak Number 7 Perylene Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.09 | 5.15 ng | 229660 | Perylene-d12 | 15.20 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Perylene | 252 | C20H12 | 000198-55-0 | 99 |
| 2 | Benzo[e]pyrene | 252 | C20H12 | 000192-97-2 | 97 |
| 3 | Benz[e]acephenanthrylene | 252 | C20H12 | 000205-99-2 | 97 |
| 4 | Benzo[k]fluoranthene | 252 | C20H12 | 000207-08-9 | 93 |
| 5 | Benzo[a]pyrene | 252 | C20H12 | 000050-32-8 | 89 |



Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF091317\
Data File : BF098507.D
Acq On : 13 Sep 2017 23:32
Operator : SJ/JU
Sample : I5160-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** G-7-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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... | 4.85 | 7.9 | ng | 413670 | 1 | 6.66 | 1043300 | 20.0 |
| unknown6.43 | 6.43 | 89.7 | ng | 4678710 | 1 | 6.66 | 1043300 | 20.0 |
| 2-Hydroxy-iso-but... | 8.50 | 3.7 | ng | 250782 | 2 | 7.94 | 1342310 | 20.0 |
| Benzophenone | 10.40 | 11.3 | ng | 750289 | 3 | 9.69 | 1327170 | 20.0 |
| Heptadecyl triflu... | 13.65 | 4.4 | ng | 289467 | 5 | 13.80 | 1316830 | 20.0 |
| Perylene | 15.09 | 5.2 | ng | 229660 | 6 | 15.20 | 892461 | 20.0 |