LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF103017\
Data File : BF099969.D
Acq On : 30 Oct 2017 19:29
Operator : SJ/JU
Sample : I6182-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT-3026

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-BF102317.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 | 4.998 | 492 | 495 | 511 | rBV | 170699 | 263905 | 13.87% | 1.636% |
| 2 | 5.410 | 562 | 565 | 589 | rBV | 1374474 | 1490194 | 78.34% | 9.239% |
| 3 | 6.433 | 735 | 739 | 757 | rBV | 1580944 | 1699374 | 89.33% | 10.536% |
| 4 | 6.563 | 757 | 761 | 773 | rVB | 1768629 | 1661638 | 87.35% | 10.302% |
| 5 | 6.786 | 796 | 799 | 808 | rBV | 614007 | 522308 | 27.46% | 3.238% |
| 6 | 6.939 | 822 | 825 | 837 | rBV | 1420625 | 1338932 | 70.38% | 8.302% |
| 7 | 7.357 | 892 | 896 | 911 | rBV | 1104249 | 1000835 | 52.61% | 6.205% |
| 8 | 8.069 | 1014 | 1017 | 1033 | rBV | 878230 | 724728 | 38.10% | 4.493% |
| 9 | 8.627 | 1109 | 1112 | 1121 | rBB | 44998 | 43087 | 2.26% | 0.267% |
| 10 | 9.145 | 1196 | 1200 | 1203 | rBV | 2323909 | 1902334 | 100.00% | 11.795% |
| 11 | 9.539 | 1264 | 1267 | 1279 | rVB | 394050 | 315005 | 16.56% | 1.953% |
| 12 | 9.827 | 1312 | 1316 | 1327 | rVB | 826940 | 754294 | 39.65% | 4.677% |
| 13 | 10.539 | 1434 | 1437 | 1442 | rBV | 175286 | 139018 | 7.31% | 0.862% |
| 14 | 10.621 | 1448 | 1451 | 1464 | rBV | 879410 | 809224 | 42.54% | 5.017% |
| 15 | 11.321 | 1566 | 1570 | 1573 | rBV | 735230 | 646220 | 33.97% | 4.007% |
| 16 | 11.345 | 1573 | 1574 | 1578 | rVB | 39673 | 27089 | 1.42% | 0.168% |
| 17 | 12.545 | 1774 | 1778 | 1783 | rBV | 44729 | 45153 | 2.37% | 0.280% |
| 18 | 12.774 | 1811 | 1817 | 1823 | rBV | 41565 | 60352 | 3.17% | 0.374% |
| 19 | 12.904 | 1835 | 1839 | 1843 | rBV | 1500390 | 1405054 | 73.86% | 8.712% |
| 20 | 13.098 | 1866 | 1872 | 1878 | rBV6 | 11119 | 22857 | 1.20% | 0.142% |
| 21 | 13.786 | 1986 | 1989 | 1997 | rBV | 117950 | 134493 | 7.07% | 0.834% |
| 22 | 13.974 | 2018 | 2021 | 2025 | rBV | 513399 | 533520 | 28.05% | 3.308% |
| 23 | 14.421 | 2094 | 2097 | 2102 | rBV5 | 16628 | 29434 | 1.55% | 0.182% |
| 24 | 14.798 | 2158 | 2161 | 2164 | rBV | 32909 | 29316 | 1.54% | 0.182% |
| 25 | 15.056 | 2199 | 2205 | 2208 | rBV3 | 32661 | 61412 | 3.23% | 0.381% |
| 26 | 15.462 | 2270 | 2274 | 2287 | rVB | 341784 | 468880 | 24.65% | 2.907% |

Sum of corrected areas: 16128656

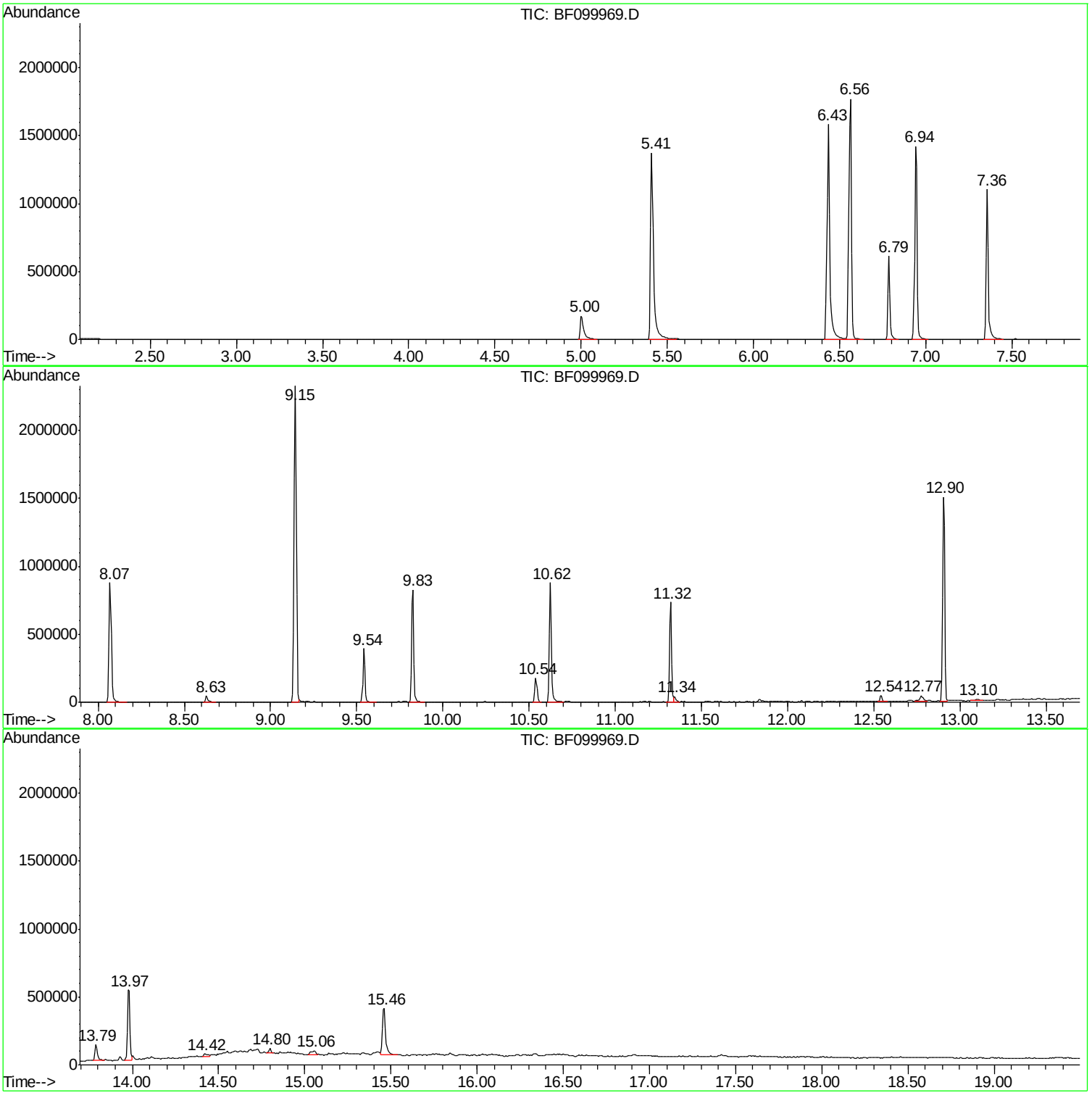
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF103017\
Data File : BF099969.D
Acq On : 30 Oct 2017 19:29
Operator : SJ/JU
Sample : I6182-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT-3026

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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:\HPCHEM1\BNA F\DATA\BF103017\
Data File : BF099969.D
Acq On : 30 Oct 2017 19:29
Operator : SJ/JU
Sample : I6182-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT-3026

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

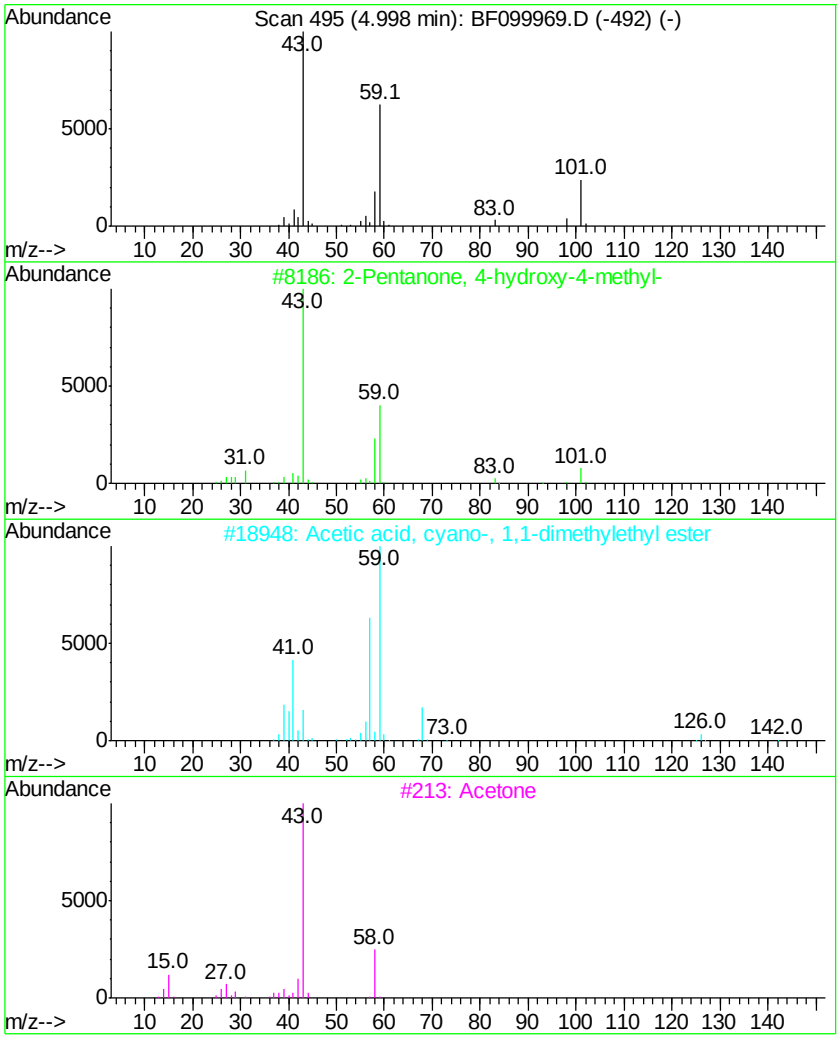
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

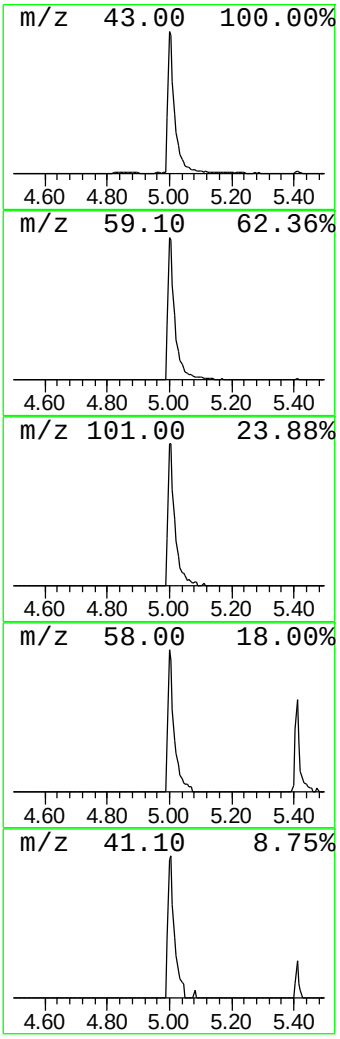
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.00 | 10.11 ng | 263905 | 1,4-Dichlorobenzene-d4 | 6.79 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 3 | Acetone | 58 | C3H6O | 000067-64-1 | 9 |
| 4 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 5 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF103017\
Data File : BF099969.D
Acq On : 30 Oct 2017 19:29
Operator : SJ/JU
Sample : I6182-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT-3026

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

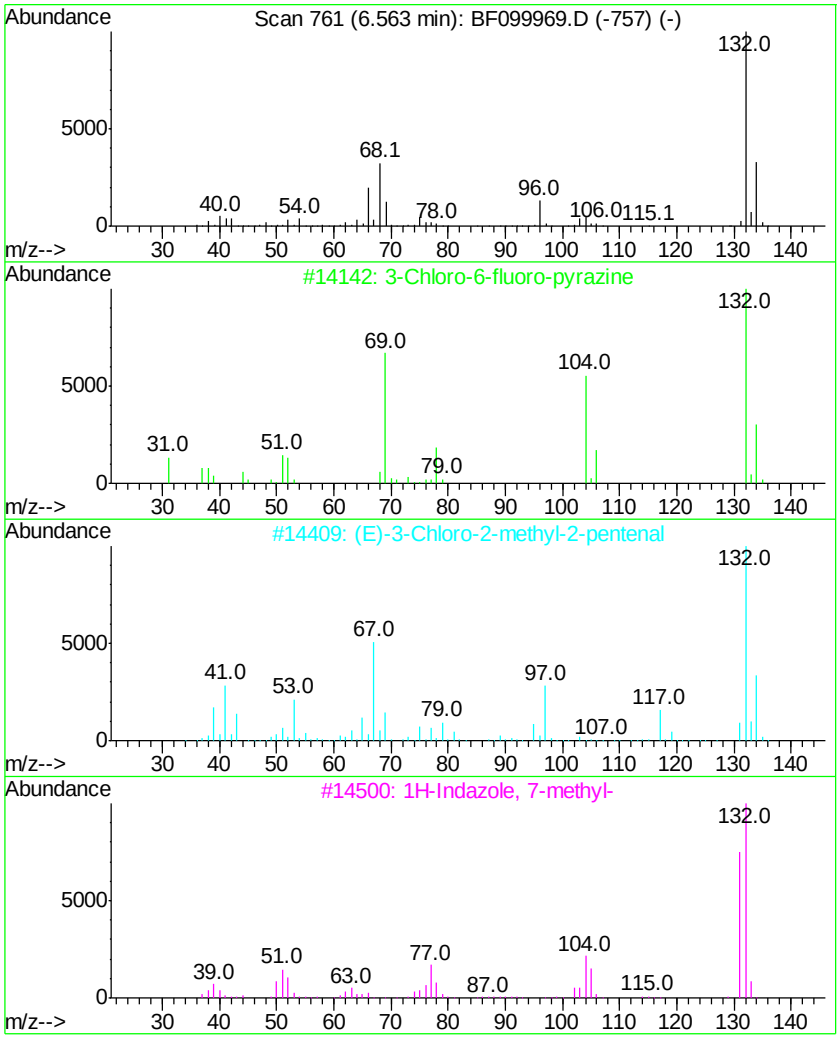
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

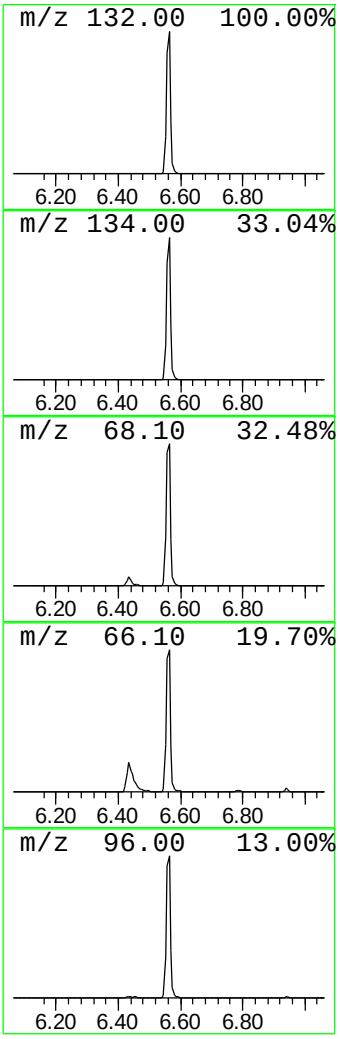
**********

Peak Number 2 unknown6.56 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.56 | 63.63 ng | 1661640 | 1,4-Dichlorobenzene-d4 | 6.79 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 38 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 17 |
| 3 | 1H-Indazole, 7-methyl- | 132 | C8H8N2 | 1000316-00-7 | 10 |
| 4 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |
| 5 | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF103017\
Data File : BF099969.D
Acq On : 30 Oct 2017 19:29
Operator : SJ/JU
Sample : I6182-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT-3026

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

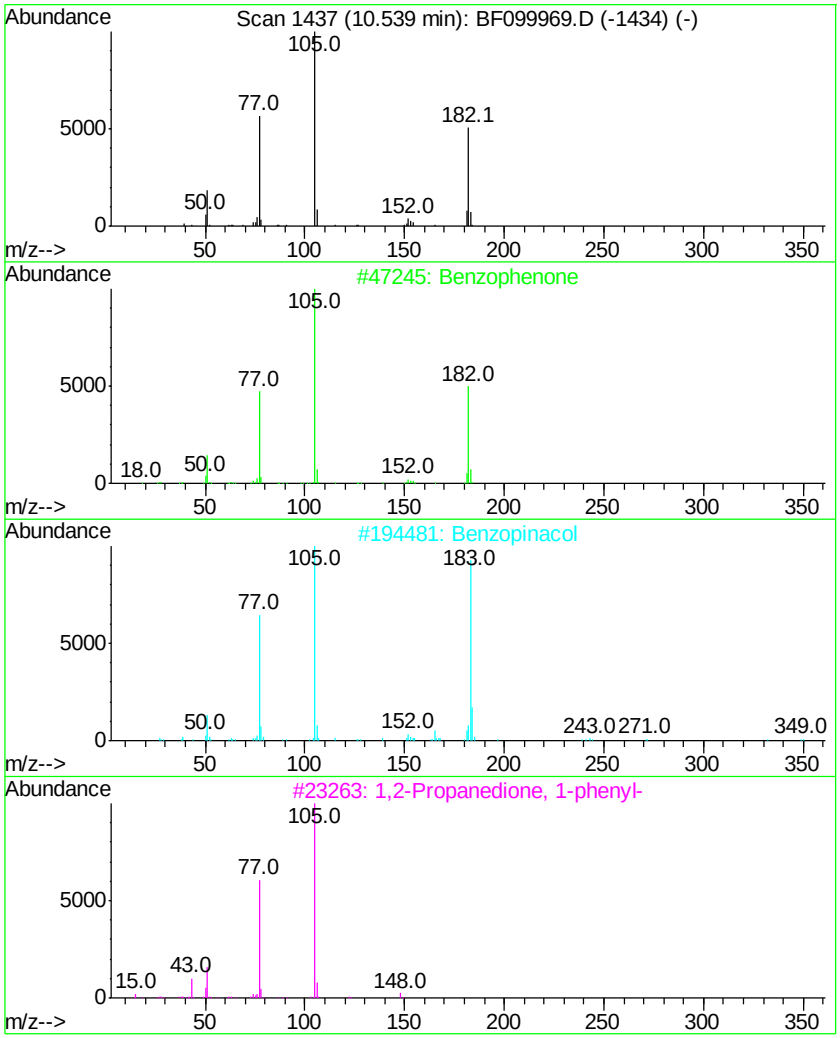
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

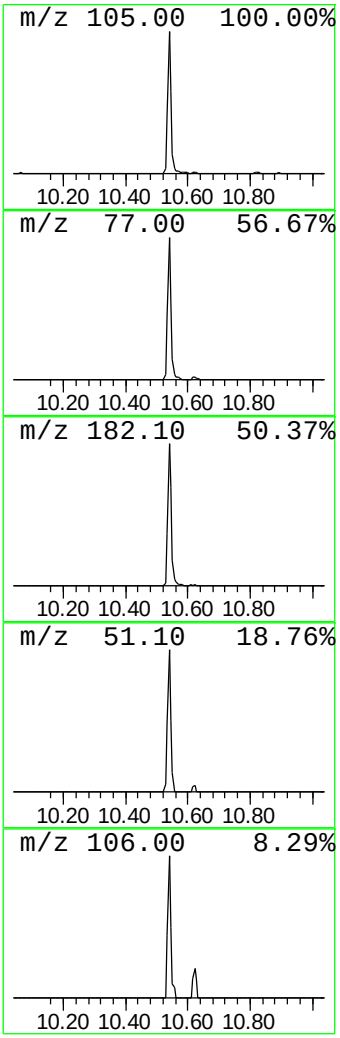
**********

Peak Number 4 Benzophenone Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.54 | 3.69 ng | 139018 | Acenaphthene-d10 | 9.83 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzophenone | 182 | C13H10O | 000119-61-9 | 97 |
| 2 | Benzopinacol | 366 | C26H22O2 | 000464-72-2 | 50 |
| 3 | 1,2-Propanedione, 1-phenyl- | 148 | C9H8O2 | 000579-07-7 | 43 |
| 4 | Acetophenone, 2-chloro- | 154 | C8H7ClO | 000532-27-4 | 43 |
| 5 | 1-Propanone, 2-bromo-1-phenyl- | 212 | C9H9BrO | 002114-00-3 | 43 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF103017\
Data File : BF099969.D
Acq On : 30 Oct 2017 19:29
Operator : SJ/JU
Sample : I6182-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT-3026

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

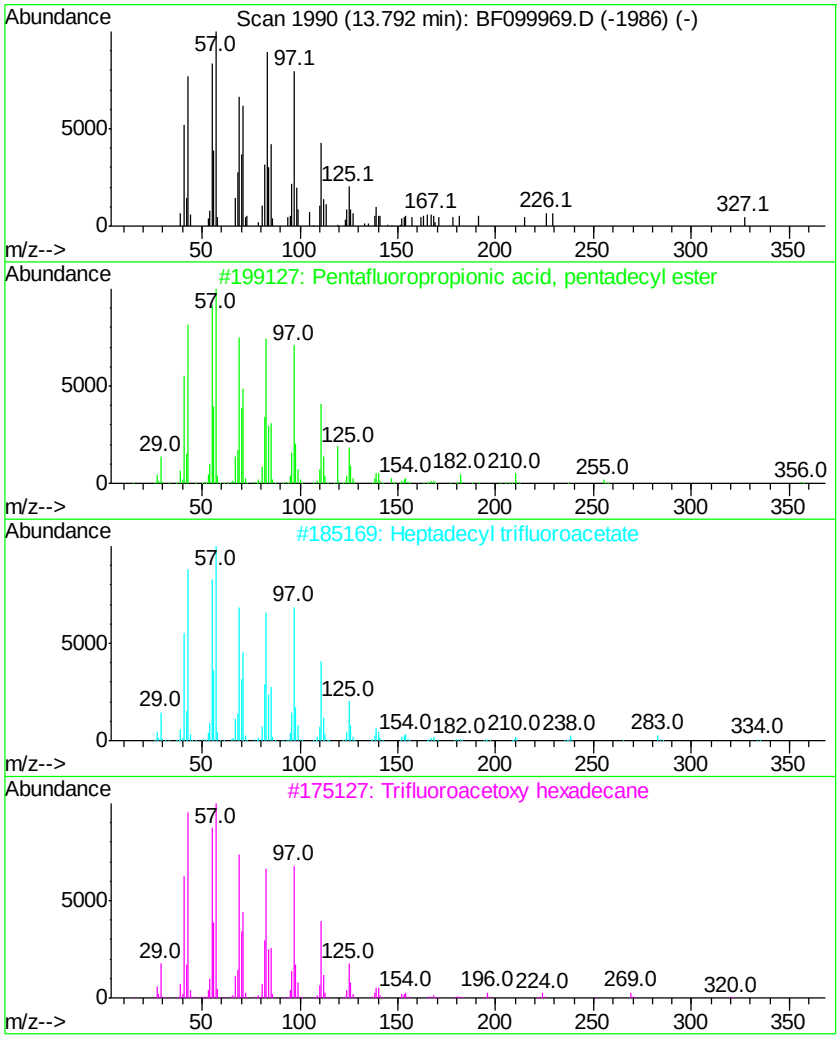
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

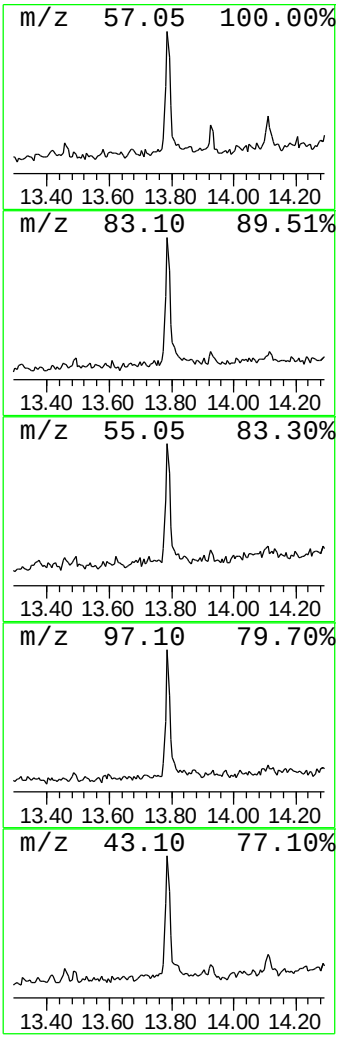
**********

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.79 | 5.04 ng | 134493 | Chrysene-d12 | 13.98 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1 | 95 |
| 2 | Heptadecyl trifluoroacetate | 352 | C19H35F3O2 | 1000351-87-0 | 95 |
| 3 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 95 |
| 4 | Pentafluoropropionic acid, hexad... | 388 | C19H33F5O2 | 006222-07-7 | 94 |
| 5 | Heptafluorobutyric acid, hexadec... | 438 | C20H33F7O2 | 006385-15-5 | 94 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF103017\
Data File : BF099969.D
Acq On : 30 Oct 2017 19:29
Operator : SJ/JU
Sample : I6182-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT-3026

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

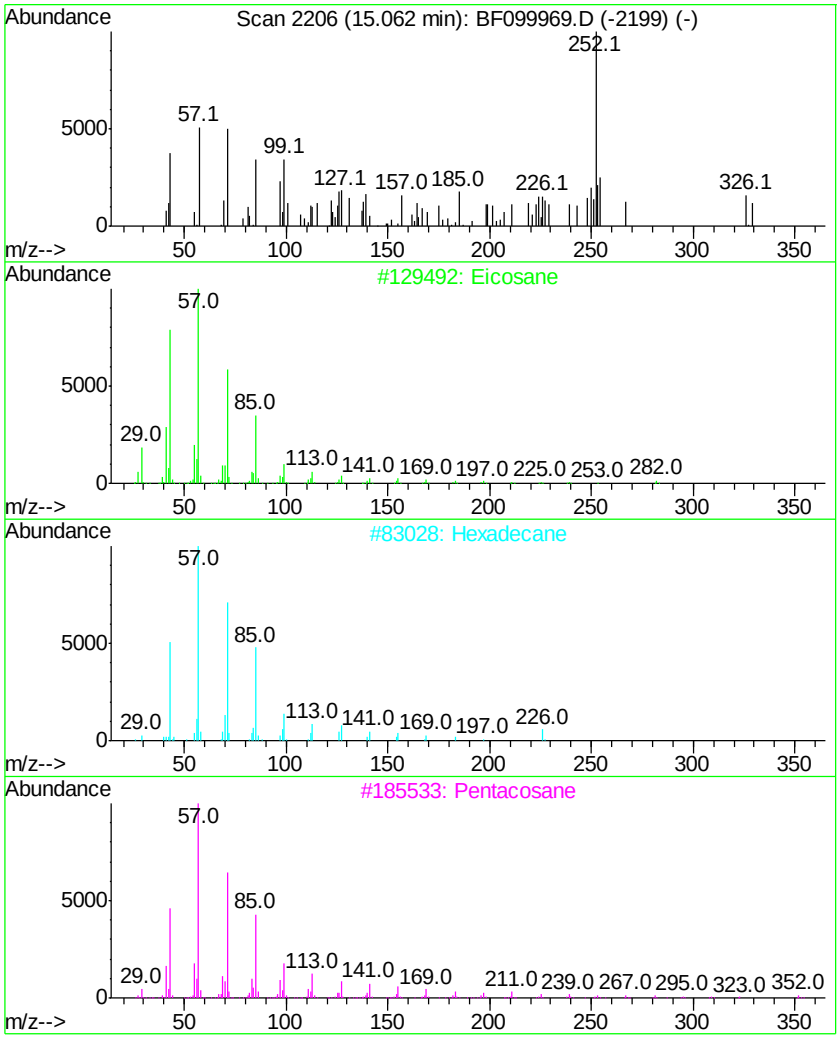
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

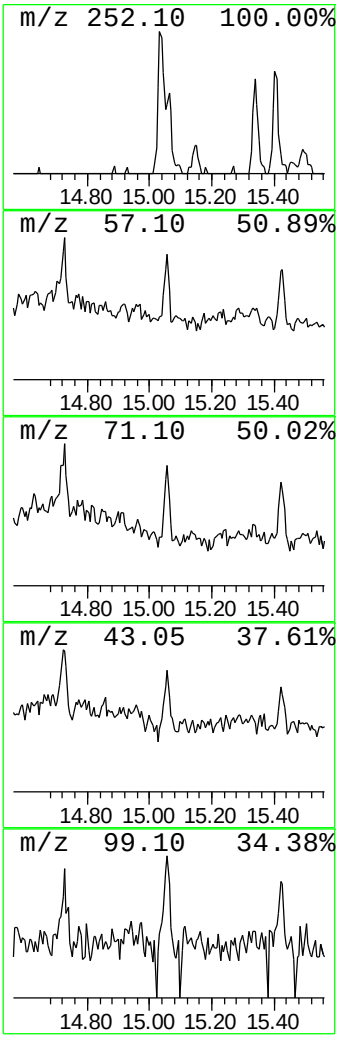
**********

Peak Number 7 Eicosane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.06 | 2.62 ng | 61412 | Perylene-d12 | 15.46 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 55 |
| 2 | Hexadecane | 226 | C16H34 | 000544-76-3 | 50 |
| 3 | Pentacosane | 352 | C25H52 | 000629-99-2 | 43 |
| 4 | Heptadecane, 9-hexyl- | 324 | C23H48 | 055124-79-3 | 43 |
| 5 | Octadecane | 254 | C18H38 | 000593-45-3 | 43 |



# Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF103017\
Data File : BF099969.D
Acq On : 30 Oct 2017 19:29
Operator : SJ/JU
Sample : I6182-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** RT-3026

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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... | 5.00 | 10.1 | ng | 263905 | 1 | 6.79 | 522308 | 20.0 |
| unknown6.56 | 6.56 | 63.6 | ng | 1661640 | 1 | 6.79 | 522308 | 20.0 |
| Benzophenone | 10.54 | 3.7 | ng | 139018 | 3 | 9.83 | 754294 | 20.0 |
| Pentafluoropropio... | 13.79 | 5.0 | ng | 134493 | 5 | 13.98 | 533520 | 20.0 |
| Eicosane | 15.06 | 2.6 | ng | 61412 | 6 | 15.46 | 468880 | 20.0 |