LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010819\
Data File : BF111919.D
Acq On : 8 Jan 2019 20:44
Operator : JU/SJ
Sample : K1044-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CPSB-08(20-25)

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-BF010719.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 | 2.199 | 14 | 19 | 28 | rVB | 88352 | 127405 | 4.60% | 0.434% |
| 2 | 5.104 | 508 | 513 | 520 | rVB | 132781 | 149895 | 5.42% | 0.511% |
| 3 | 5.487 | 574 | 578 | 580 | rBV | 89059 | 111057 | 4.01% | 0.379% |
| 4 | 5.522 | 580 | 584 | 600 | rVB | 2800318 | 2539549 | 91.75% | 8.658% |
| 5 | 6.528 | 750 | 755 | 766 | rBV | 2793099 | 2768030 | 100.00% | 9.437% |
| 6 | 6.663 | 773 | 778 | 781 | rBV | 2555193 | 2458713 | 88.83% | 8.382% |
| 7 | 6.886 | 812 | 816 | 822 | rBV | 908123 | 782790 | 28.28% | 2.669% |
| 8 | 7.045 | 838 | 843 | 846 | rBV | 2219043 | 2035942 | 73.55% | 6.941% |
| 9 | 7.292 | 881 | 885 | 894 | rBV | 438683 | 386046 | 13.95% | 1.316% |
| 10 | 7.439 | 904 | 910 | 914 | rBV | 1603820 | 1551325 | 56.04% | 5.289% |
| 11 | 8.169 | 1030 | 1034 | 1037 | rBV | 948100 | 779352 | 28.16% | 2.657% |
| 12 | 9.239 | 1212 | 1216 | 1219 | rBV | 3199108 | 2609767 | 94.28% | 8.897% |
| 13 | 9.510 | 1254 | 1262 | 1266 | rBV5 | 23774 | 34749 | 1.26% | 0.118% |
| 14 | 9.627 | 1279 | 1282 | 1287 | rVB | 277086 | 235318 | 8.50% | 0.802% |
| 15 | 9.810 | 1310 | 1313 | 1316 | rBV2 | 39216 | 44597 | 1.61% | 0.152% |
| 16 | 9.922 | 1328 | 1332 | 1336 | rBV | 942162 | 785267 | 28.37% | 2.677% |
| 17 | 10.286 | 1392 | 1394 | 1398 | rBV3 | 29637 | 35201 | 1.27% | 0.120% |
| 18 | 10.710 | 1462 | 1466 | 1470 | rBV | 1630824 | 1332192 | 48.13% | 4.542% |
| 19 | 10.786 | 1475 | 1479 | 1482 | rVV | 587396 | 523475 | 18.91% | 1.785% |
| 20 | 10.821 | 1482 | 1485 | 1486 | rVV2 | 48214 | 45587 | 1.65% | 0.155% |
| 21 | 10.839 | 1486 | 1488 | 1496 | rVV | 60220 | 61409 | 2.22% | 0.209% |
| 22 | 10.904 | 1496 | 1499 | 1504 | rVB5 | 26132 | 36540 | 1.32% | 0.125% |
| 23 | 11.304 | 1564 | 1567 | 1570 | rVB | 108925 | 95562 | 3.45% | 0.326% |
| 24 | 11.410 | 1581 | 1585 | 1588 | rBV | 804408 | 714538 | 25.81% | 2.436% |
| 25 | 11.433 | 1588 | 1589 | 1591 | rVV2 | 81853 | 65189 | 2.36% | 0.222% |
| 26 | 11.463 | 1591 | 1594 | 1596 | rVB | 86874 | 76173 | 2.75% | 0.260% |
| 27 | 11.621 | 1618 | 1621 | 1624 | rBV3 | 44383 | 48330 | 1.75% | 0.165% |
| 28 | 11.798 | 1648 | 1651 | 1653 | rBV | 39842 | 32645 | 1.18% | 0.111% |
| 29 | 11.933 | 1670 | 1674 | 1679 | rBV | 149662 | 145689 | 5.26% | 0.497% |
| 30 | 12.392 | 1749 | 1752 | 1757 | rBV6 | 21337 | 35099 | 1.27% | 0.120% |
| 31 | 12.445 | 1758 | 1761 | 1765 | rVV5 | 38096 | 49148 | 1.78% | 0.168% |
| 32 | 12.480 | 1765 | 1767 | 1769 | rVV2 | 114582 | 106864 | 3.86% | 0.364% |
| 33 | 12.504 | 1769 | 1771 | 1776 | rVB | 215651 | 177294 | 6.41% | 0.604% |
| 34 | 12.621 | 1789 | 1791 | 1796 | rBV2 | 22788 | 33364 | 1.21% | 0.114% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010819\
Data File : BF111919.D
Acq On : 8 Jan 2019 20:44
Operator : JU/SJ
Sample : K1044-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CPSB-08(20-25)

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-BF010719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 12.663 | 1796 | 1798 | 1804 | rVB2 | 61871 | 63658 | 2.30% | 0.217% |
| 36 | 12.715 | 1804 | 1807 | 1811 | rBV5 | 29036 | 37162 | 1.34% | 0.127% |
| 37 | 12.992 | 1848 | 1854 | 1857 | rBV | 2576293 | 2235189 | 80.75% | 7.620% |
| 38 | 13.133 | 1875 | 1878 | 1881 | rBV | 82434 | 91122 | 3.29% | 0.311% |
| 39 | 13.221 | 1891 | 1893 | 1896 | rBV | 71415 | 74943 | 2.71% | 0.255% |
| 40 | 13.562 | 1949 | 1951 | 1953 | rBV | 54049 | 37574 | 1.36% | 0.128% |
| 41 | 13.680 | 1968 | 1971 | 1974 | rBV | 465724 | 384519 | 13.89% | 1.311% |
| 42 | 13.886 | 2002 | 2006 | 2013 | rVB2 | 438202 | 570908 | 20.63% | 1.946% |
| 43 | 13.951 | 2014 | 2017 | 2019 | rBV4 | 62882 | 95078 | 3.43% | 0.324% |
| 44 | 14.051 | 2030 | 2034 | 2037 | rVB | 840115 | 794442 | 28.70% | 2.708% |
| 45 | 14.209 | 2058 | 2061 | 2066 | rBV | 113827 | 102343 | 3.70% | 0.349% |
| 46 | 14.333 | 2078 | 2082 | 2085 | rBV | 568979 | 508690 | 18.38% | 1.734% |
| 47 | 14.515 | 2110 | 2113 | 2119 | rVB | 534986 | 518629 | 18.74% | 1.768% |
| 48 | 14.904 | 2176 | 2179 | 2180 | rBV | 59351 | 53527 | 1.93% | 0.182% |
| 49 | 14.968 | 2187 | 2190 | 2195 | rVB | 192871 | 221353 | 8.00% | 0.755% |
| 50 | 15.133 | 2216 | 2218 | 2219 | rBV2 | 53060 | 42978 | 1.55% | 0.147% |
| 51 | 15.168 | 2220 | 2224 | 2227 | rVV | 393256 | 482348 | 17.43% | 1.644% |
| 52 | 15.533 | 2282 | 2286 | 2296 | rVB | 436858 | 840019 | 30.35% | 2.864% |
| 53 | 15.633 | 2298 | 2303 | 2304 | rBV5 | 66246 | 115003 | 4.15% | 0.392% |
| 54 | 15.998 | 2362 | 2365 | 2370 | rVB | 162721 | 232812 | 8.41% | 0.794% |
| 55 | 16.051 | 2370 | 2374 | 2378 | rBV5 | 98772 | 173877 | 6.28% | 0.593% |
| 56 | 16.351 | 2423 | 2425 | 2427 | rBV3 | 60180 | 65385 | 2.36% | 0.223% |
| 57 | 16.515 | 2447 | 2453 | 2457 | rBV3 | 103017 | 239123 | 8.64% | 0.815% |
| 58 | 16.674 | 2478 | 2480 | 2482 | rBV2 | 58148 | 56328 | 2.03% | 0.192% |
| 59 | 16.962 | 2527 | 2529 | 2531 | rBV2 | 81711 | 107510 | 3.88% | 0.367% |
| 60 | 17.709 | 2650 | 2656 | 2657 | rBV5 | 105190 | 173883 | 6.28% | 0.593% |

Sum of corrected areas: 29332504

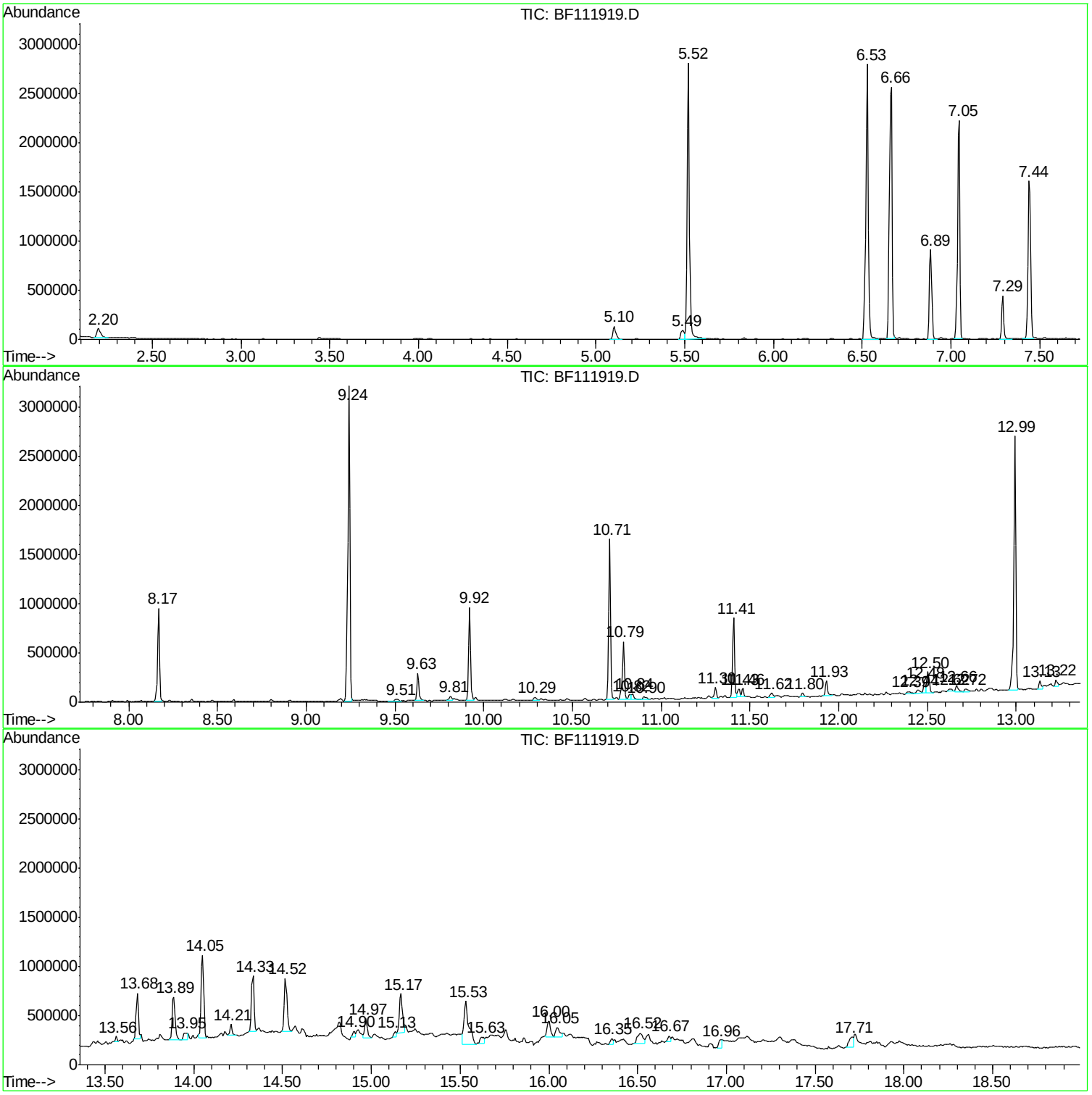
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010819\
Data File : BF111919.D
Acq On : 8 Jan 2019 20:44
Operator : JU/SJ
Sample : K1044-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CPSB-08(20-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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\BF010819\
Data File : BF111919.D
Acq On : 8 Jan 2019 20:44
Operator : JU/SJ
Sample : K1044-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CPSB-08(20-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

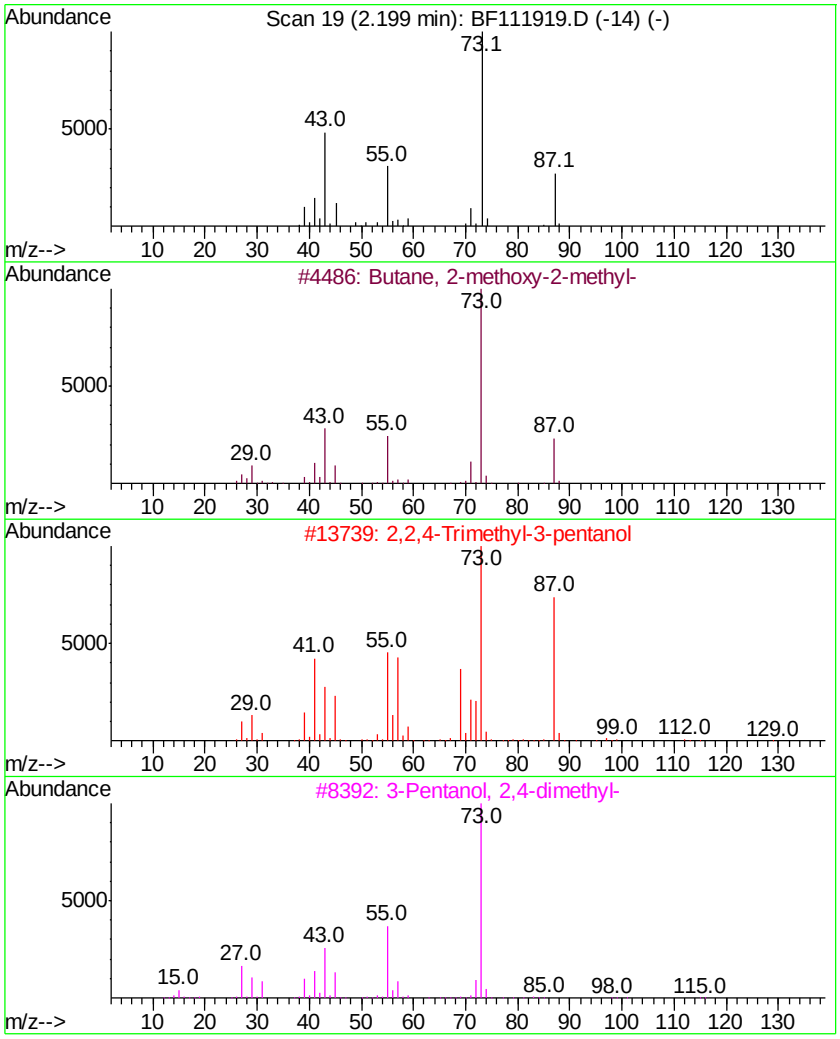
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

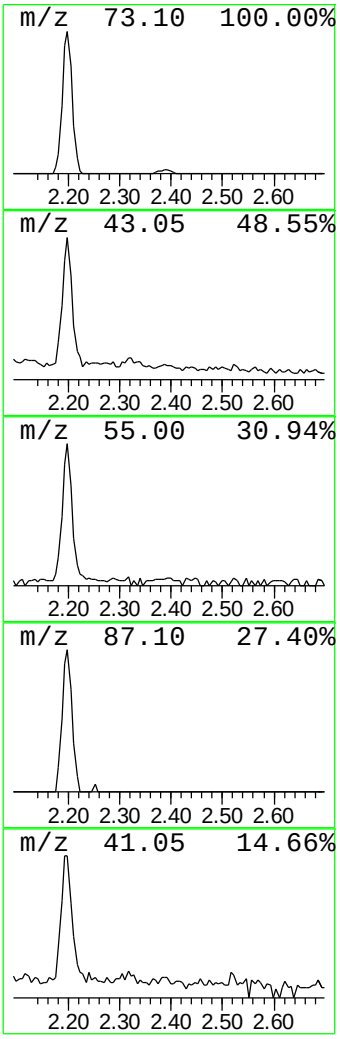
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 17

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.20 | 3.26 ng | 127405 | 1,4-Dichlorobenzene-d4 | 6.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 78 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 40 |
| 3 | 3-Pentanol, 2,4-dimethyl- | 116 | C7H16O | 000600-36-2 | 38 |
| 4 | 2-Methyl-5-hexen-3-ol | 114 | C7H14O | 032815-70-6 | 12 |
| 5 | Boronic acid, ethyl-, dimethyl e... | 102 | C4H11BO2 | 007318-82-3 | 10 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010819\
Data File : BF111919.D
Acq On : 8 Jan 2019 20:44
Operator : JU/SJ
Sample : K1044-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CPSB-08(20-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

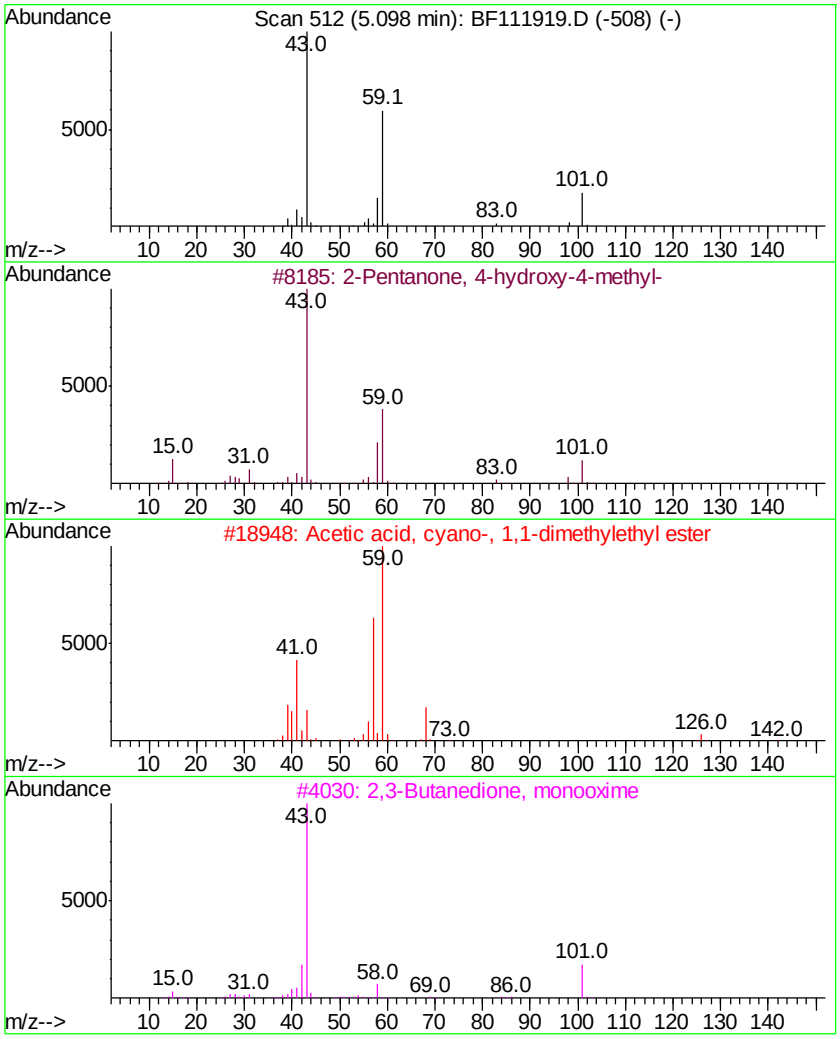
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

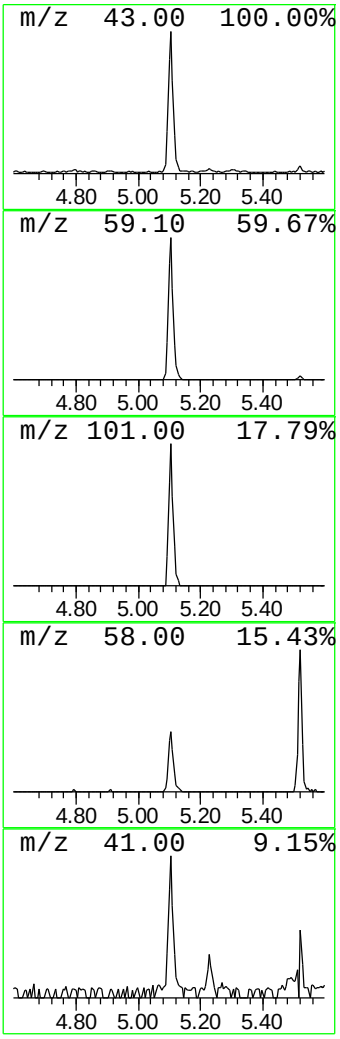
**********

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.10 | 3.83 ng | 149895 | 1,4-Dichlorobenzene-d4 | 6.89 |

| 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 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 4 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |
| 5 | Silane, trimethyl- | 74 | C3H10Si | 000993-07-7 | 9 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010819\
Data File : BF111919.D
Acq On : 8 Jan 2019 20:44
Operator : JU/SJ
Sample : K1044-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CPSB-08(20-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

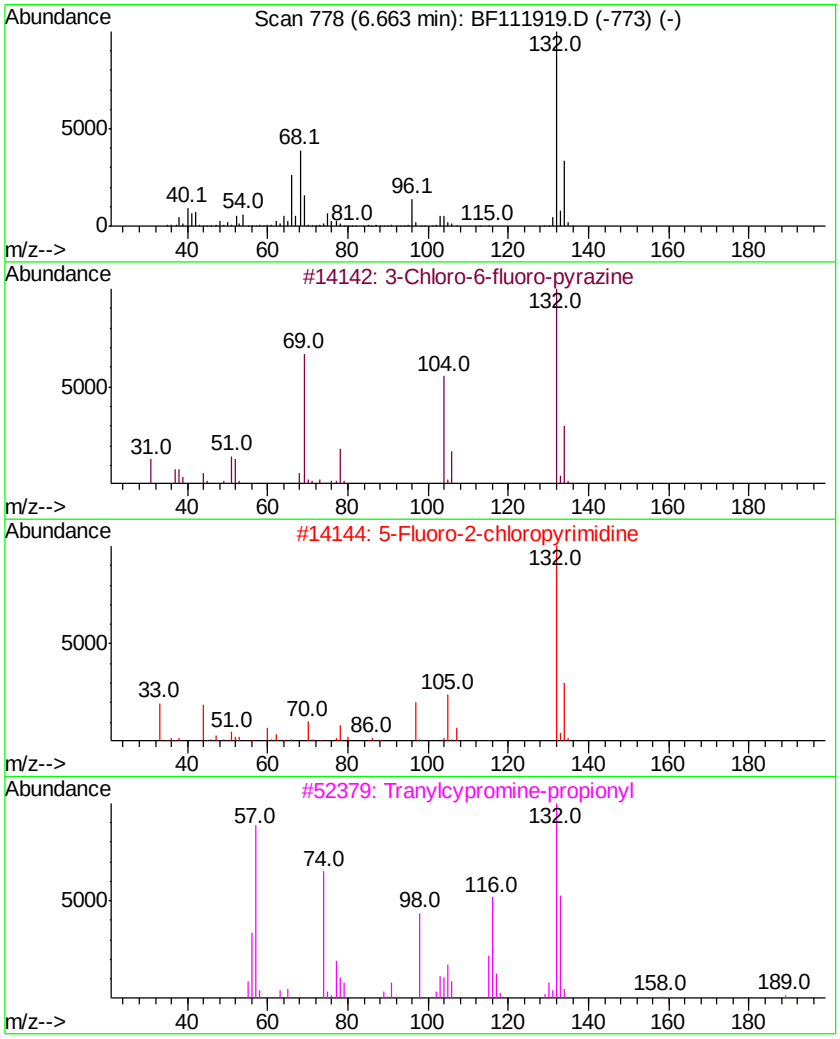
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

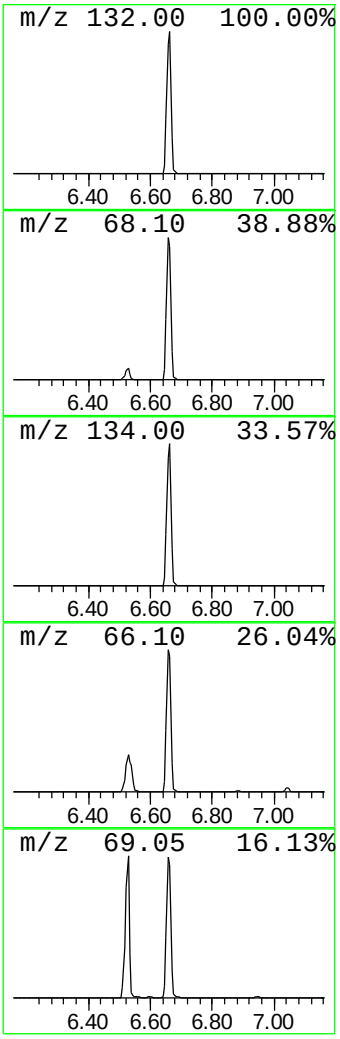
**********

Peak Number 3 unknown6.66 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.66 | 62.82 ng | 2458710 | 1,4-Dichlorobenzene-d4 | 6.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 4 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 12 |
| 5 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010819\
Data File : BF111919.D
Acq On : 8 Jan 2019 20:44
Operator : JU/SJ
Sample : K1044-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CPSB-08(20-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

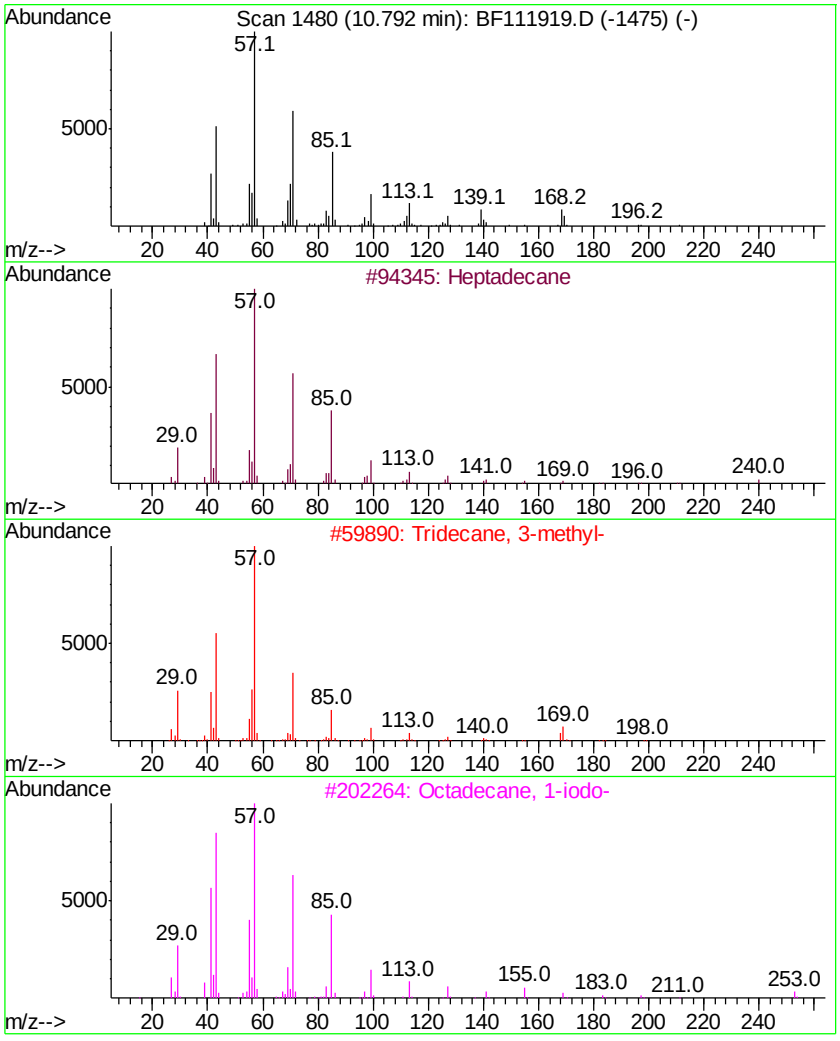
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

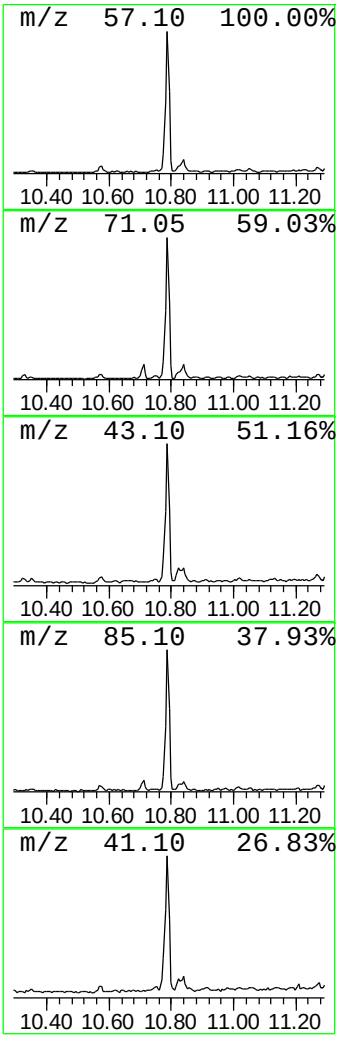
**********

Peak Number 5 Heptadecane Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.79 | 14.65 ng | 523475 | Phenanthrene-d10 | 11.41 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane | 240 | C17H36 | 000629-78-7 | 72 |
| 2 | Tridecane, 3-methyl- | 198 | C14H30 | 006418-41-3 | 72 |
| 3 | Octadecane, 1-iodo- | 380 | C18H37I | 000629-93-6 | 64 |
| 4 | Tridecane, 5-propyl- | 226 | C16H34 | 055045-11-9 | 64 |
| 5 | 2-Bromotetradecane | 276 | C14H29Br | 074036-95-6 | 64 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010819\
Data File : BF111919.D
Acq On : 8 Jan 2019 20:44
Operator : JU/SJ
Sample : K1044-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CPSB-08(20-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

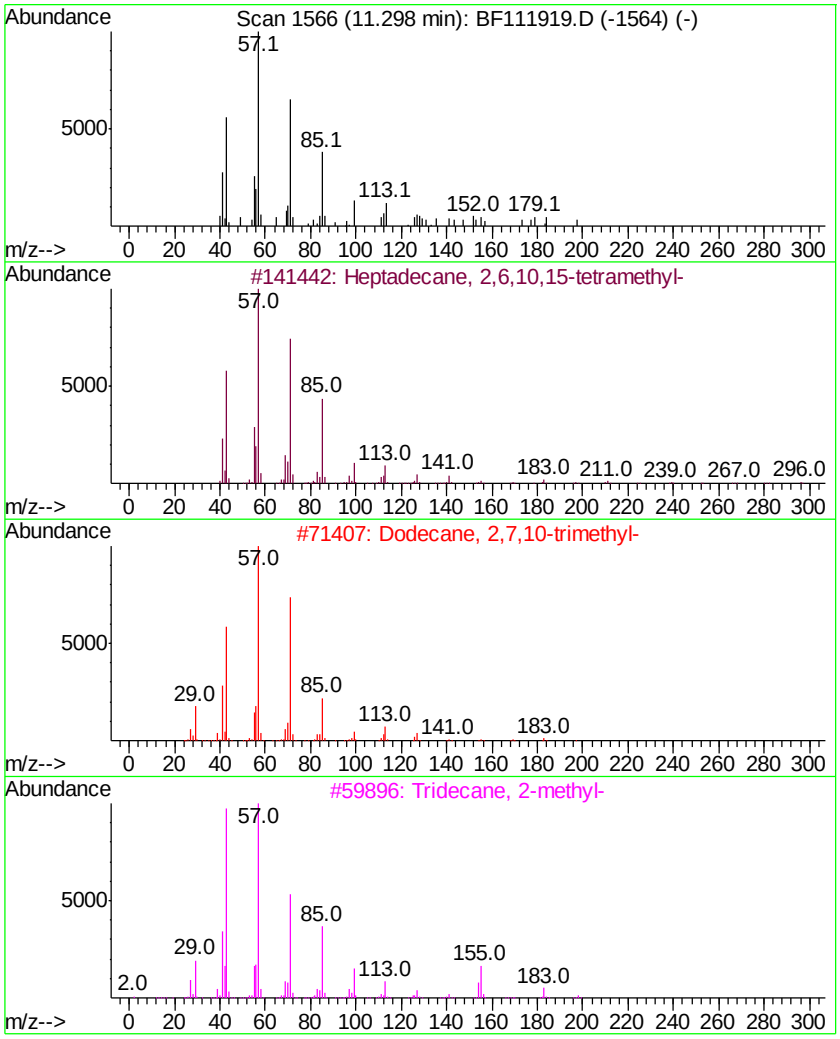
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

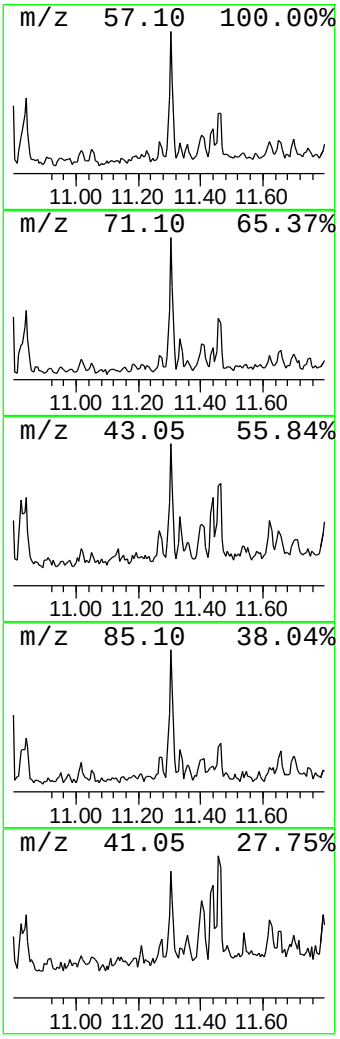
**********

Peak Number 6 Heptadecane, 2,6,10,15-tetr... Concentration Rank 20

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.30 | 2.67 ng | 95562 | Phenanthrene-d10 | 11.41 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane, 2,6,10,15-tetramethyl- | 296 | C21H44 | 054833-48-6 | 83 |
| 2 | Dodecane, 2,7,10-trimethyl- | 212 | C15H32 | 074645-98-0 | 80 |
| 3 | Tridecane, 2-methyl- | 198 | C14H30 | 001560-96-9 | 74 |
| 4 | Dodecane, 2,6,11-trimethyl- | 212 | C15H32 | 031295-56-4 | 72 |
| 5 | Heneicosane | 296 | C21H44 | 000629-94-7 | 72 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010819\
Data File : BF111919.D
Acq On : 8 Jan 2019 20:44
Operator : JU/SJ
Sample : K1044-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CPSB-08(20-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

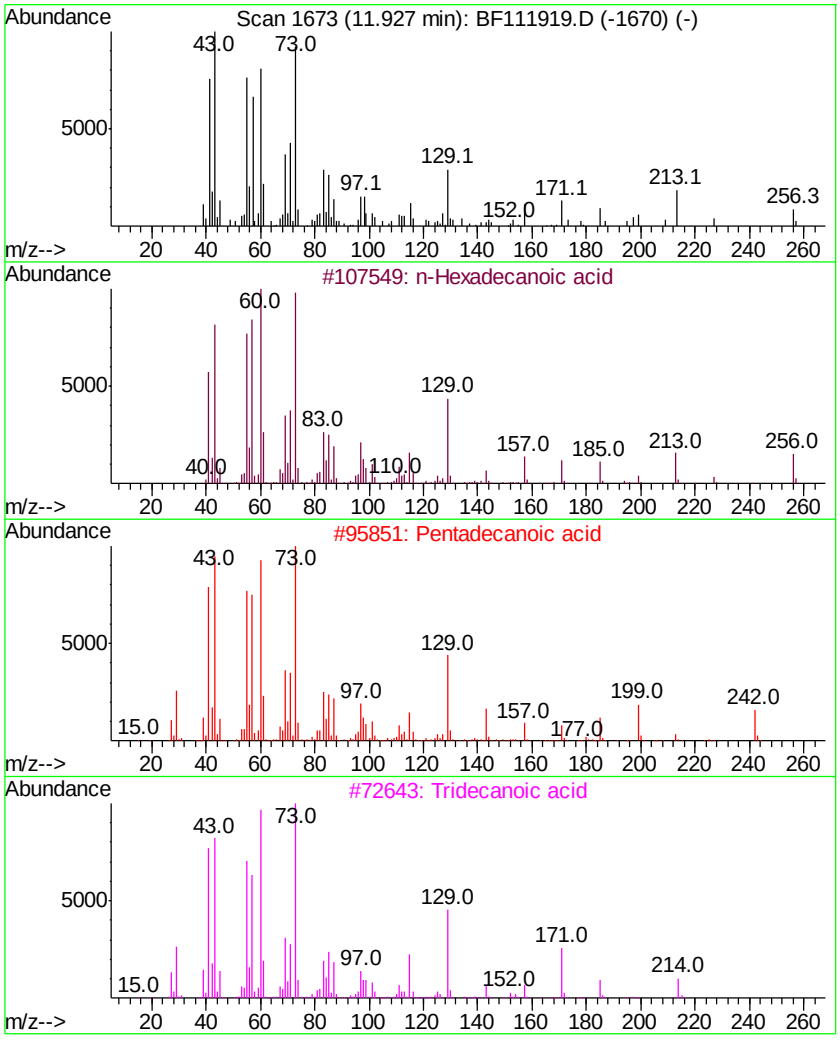
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

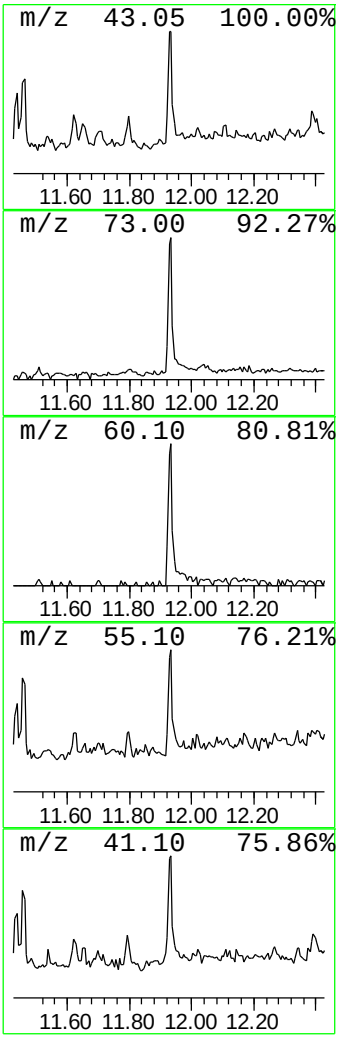
**********

Peak Number 7 n-Hexadecanoic acid Concentration Rank 15

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.93 | 4.08 ng | 145689 | Phenanthrene-d10 | 11.41 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 90 |
| 3 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 90 |
| 4 | Nonanoic acid | 158 | C9H18O2 | 000112-05-0 | 25 |
| 5 | 2-Butenoic acid, 2-methoxy-3-met... | 144 | C7H12O3 | 056009-32-6 | 18 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010819\
Data File : BF111919.D
Acq On : 8 Jan 2019 20:44
Operator : JU/SJ
Sample : K1044-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CPSB-08(20-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

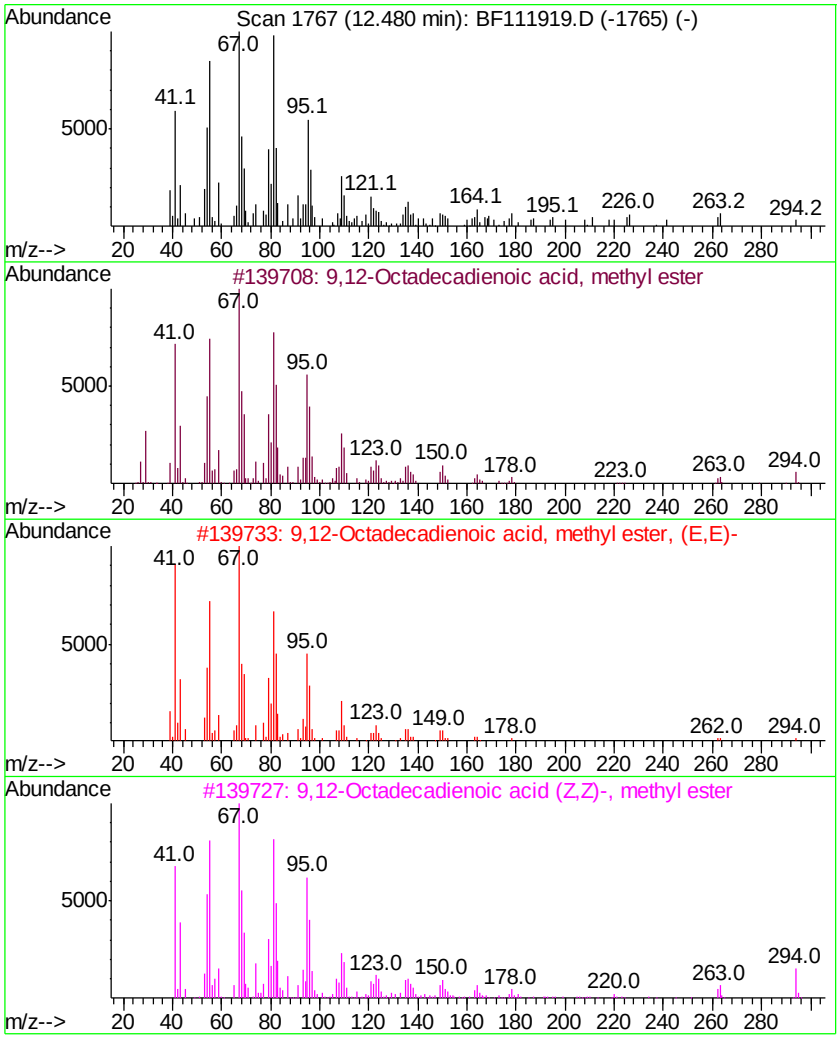
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

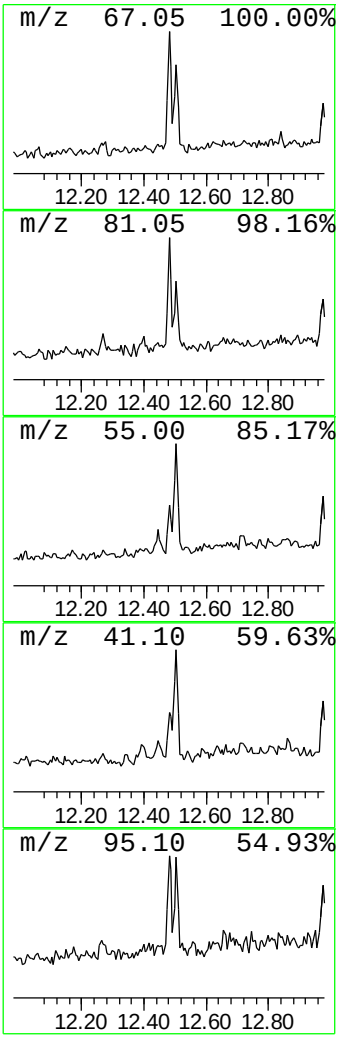
**********

Peak Number 8 9,12-Octadecadienoic acid, ... Concentration Rank 18

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.48 | 2.99 ng | 106864 | Phenanthrene-d10 | 11.41 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9,12-Octadecadienoic acid, methy... | 294 | C19H34O2 | 002462-85-3 | 99 |
| 2 | 9,12-Octadecadienoic acid, methy... | 294 | C19H34O2 | 002566-97-4 | 98 |
| 3 | 9,12-Octadecadienoic acid (Z,Z)-... | 294 | C19H34O2 | 000112-63-0 | 95 |
| 4 | 11,14-Octadecadienoic acid, meth... | 294 | C19H34O2 | 056554-61-1 | 95 |
| 5 | Bicyclo[2.2.2]octane, 2-methyl- | 124 | C9H16 | 000766-53-0 | 81 |



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Data File : BF111919.D
Acq On : 8 Jan 2019 20:44
Operator : JU/SJ
Sample : K1044-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CPSB-08(20-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

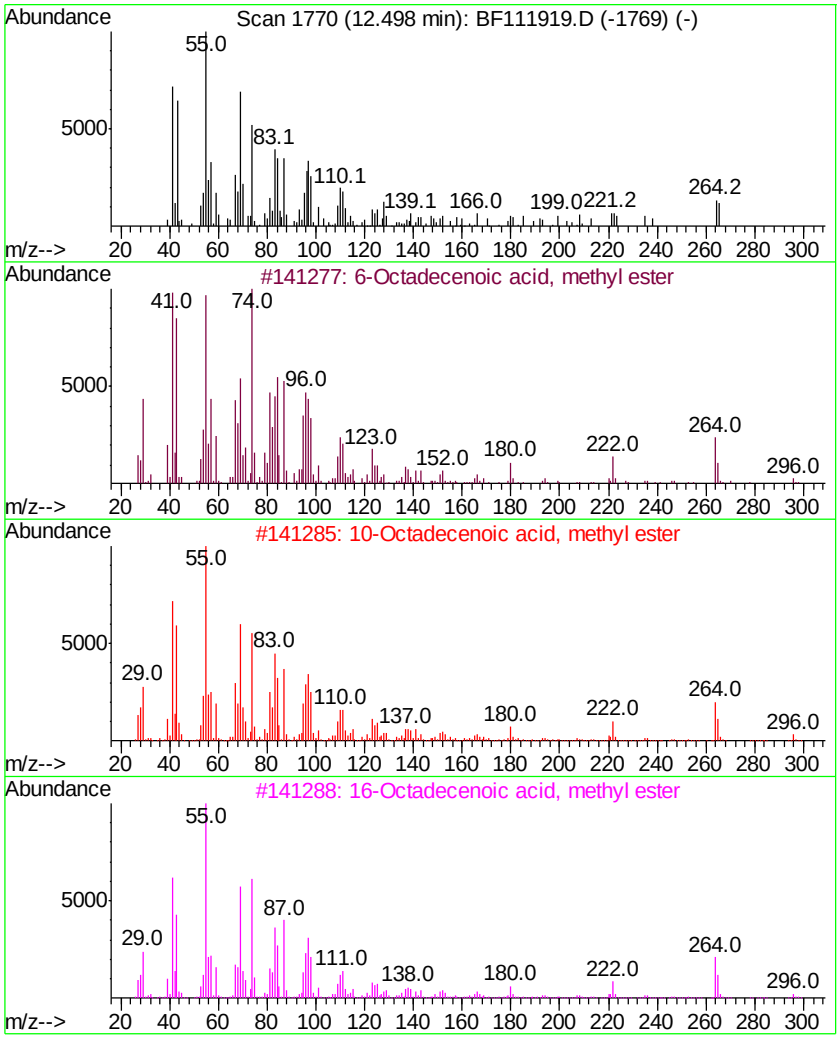
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

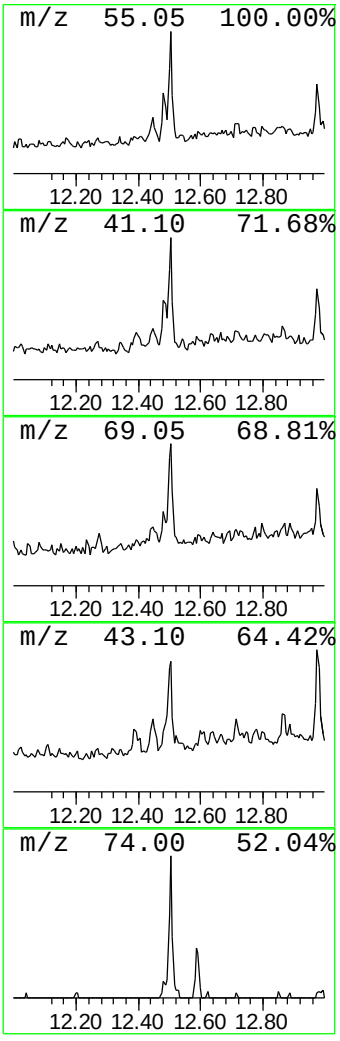
**********

Peak Number 9 6-Octadecenoic acid, methyl... Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.50 | 4.96 ng | 177294 | Phenanthrene-d10 | 11.41 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 6-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 052355-31-4 | 93 |
| 2 | 10-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 013481-95-3 | 93 |
| 3 | 16-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 056554-49-5 | 90 |
| 4 | 9-Octadecenoic acid (Z)-, methyl... | 296 | C19H36O2 | 000112-62-9 | 90 |
| 5 | 15-Octadecenoic acid, methyl ester | 296 | C19H36O2 | 004764-72-1 | 87 |



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Data File : BF111919.D
Acq On : 8 Jan 2019 20:44
Operator : JU/SJ
Sample : K1044-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CPSB-08(20-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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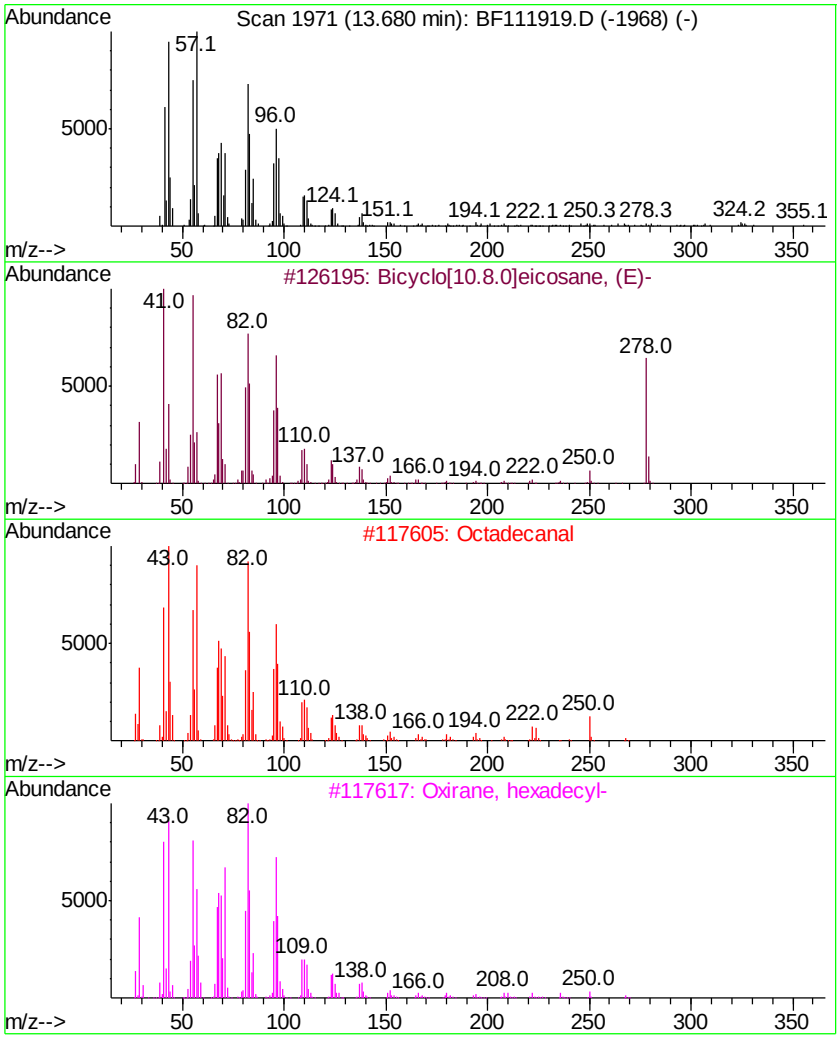
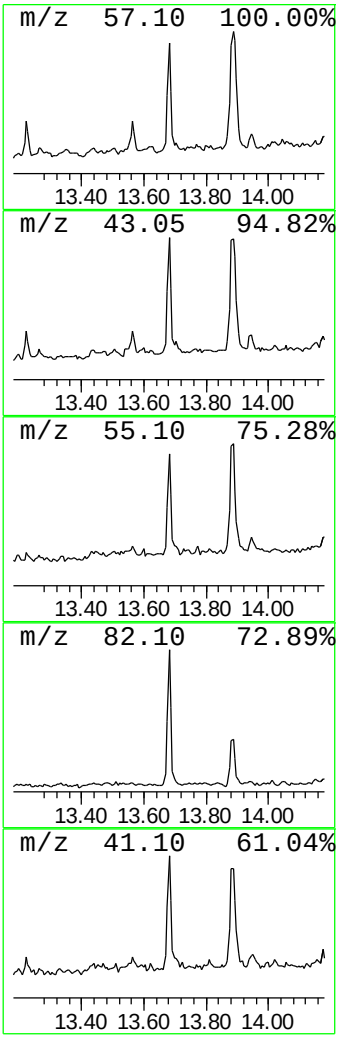
Peak Number 10 Bicyclo[10.8.0]eicosane, (E)- Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.68 | 9.68 ng | 384519 | Chrysene-d12 | 14.05 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Bicyclo[10.8.0]eicosane, (E)- | 278 | C20H38 | 1000155-85-0 | 95 |
| 2 | Octadecanal | 268 | C18H36O | 000638-66-4 | 95 |
| 3 | Oxirane, hexadecyl- | 268 | C18H36O | 007390-81-0 | 95 |
| 4 | 1,21-Docosadiene | 306 | C22H42 | 053057-53-7 | 95 |
| 5 | Z-2-Octadecen-1-ol | 268 | C18H36O | 1000131-11-0 | 93 |



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Data File : BF111919.D
Acq On : 8 Jan 2019 20:44
Operator : JU/SJ
Sample : K1044-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CPSB-08(20-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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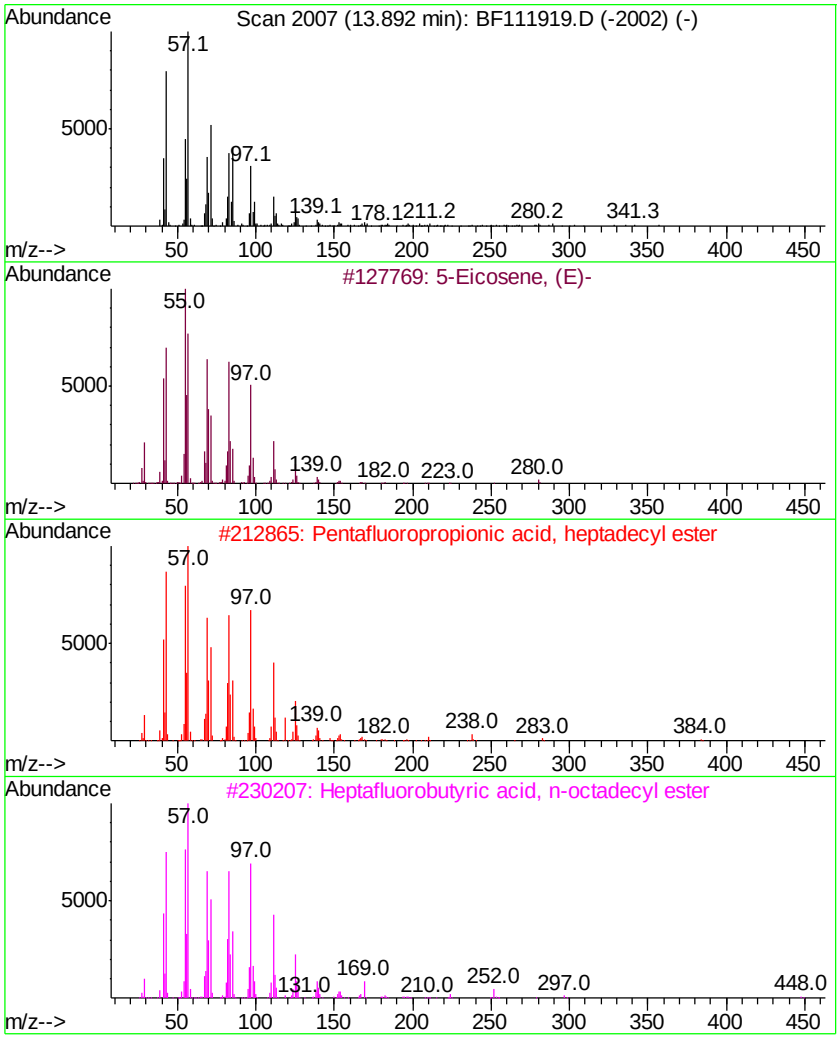
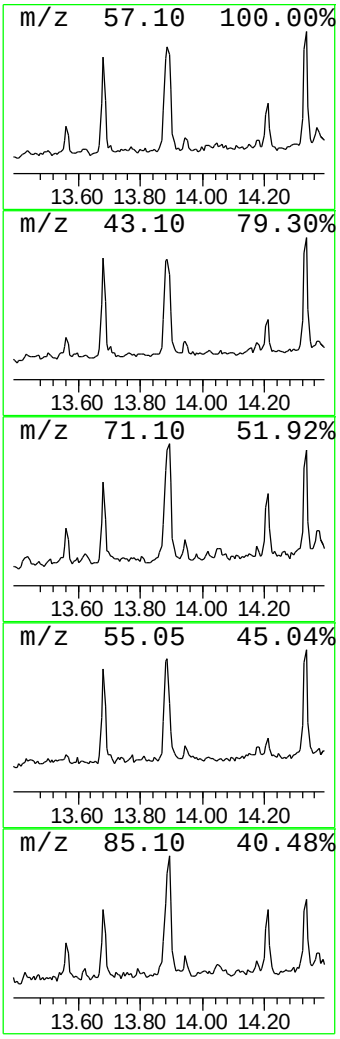
Peak Number 11 5-Eicosene, (E)- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.89 | 14.37 ng | 570908 | Chrysene-d12 | 14.05 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Eicosene, (E)- | 280 | C20H40 | 074685-30-6 | 96 |
| 2 | Pentafluoropropionic acid, hepta... | 402 | C20H35F5O2 | 959218-78-1 | 94 |
| 3 | Heptafluorobutyric acid, n-octad... | 466 | C22H37F7O2 | 000400-57-7 | 94 |
| 4 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 93 |
| 5 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 93 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010819\
Data File : BF111919.D
Acq On : 8 Jan 2019 20:44
Operator : JU/SJ
Sample : K1044-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CPSB-08(20-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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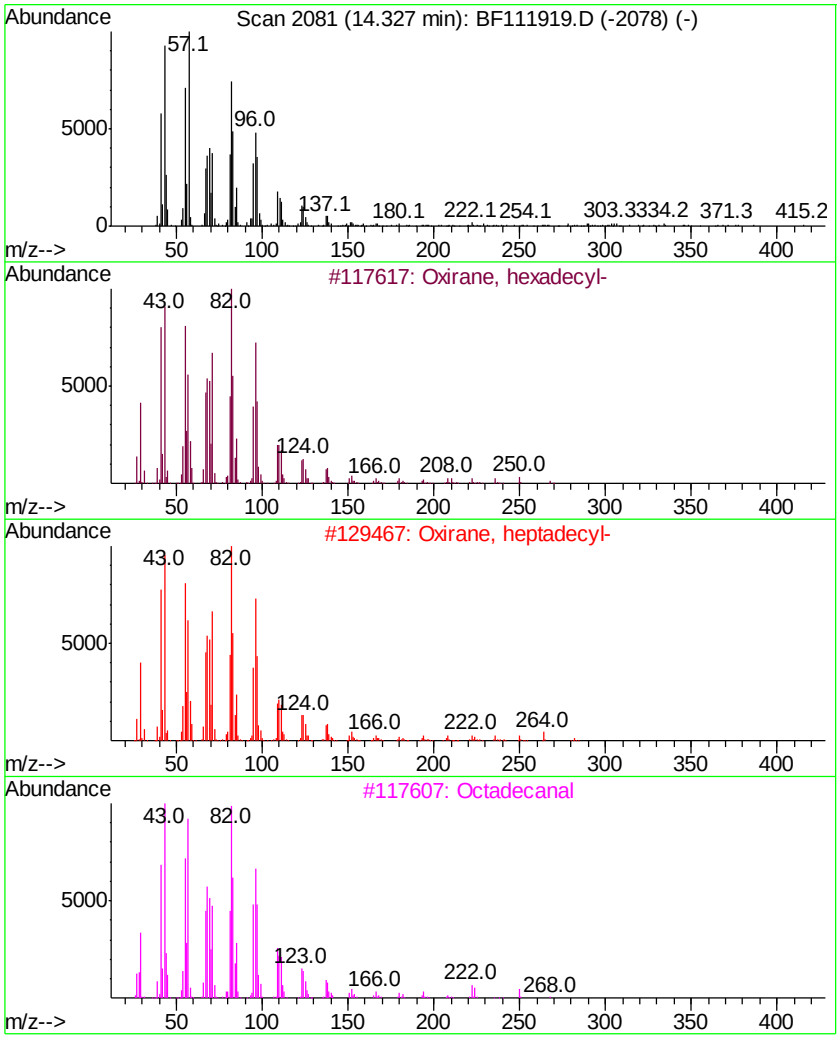
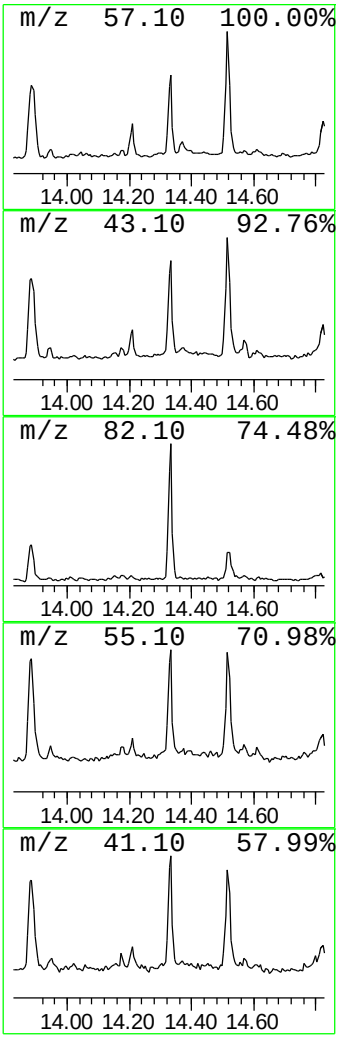
Peak Number 12 Oxirane, hexadecyl- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.33 | 12.81 ng | 508690 | Chrysene-d12 | 14.05 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Oxirane, hexadecyl- | 268 | C18H36O | 007390-81-0 | 91 |
| 2 | Oxirane, heptadecyl- | 282 | C19H38O | 067860-04-2 | 91 |
| 3 | Octadecanal | 268 | C18H36O | 000638-66-4 | 91 |
| 4 | Tetradecanal | 212 | C14H28O | 000124-25-4 | 91 |
| 5 | 17-Octadecenal | 266 | C18H34O | 056554-86-0 | 91 |



# Library Search Compound Report

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Data File : BF111919.D
Acq On : 8 Jan 2019 20:44
Operator : JU/SJ
Sample : K1044-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CPSB-08(20-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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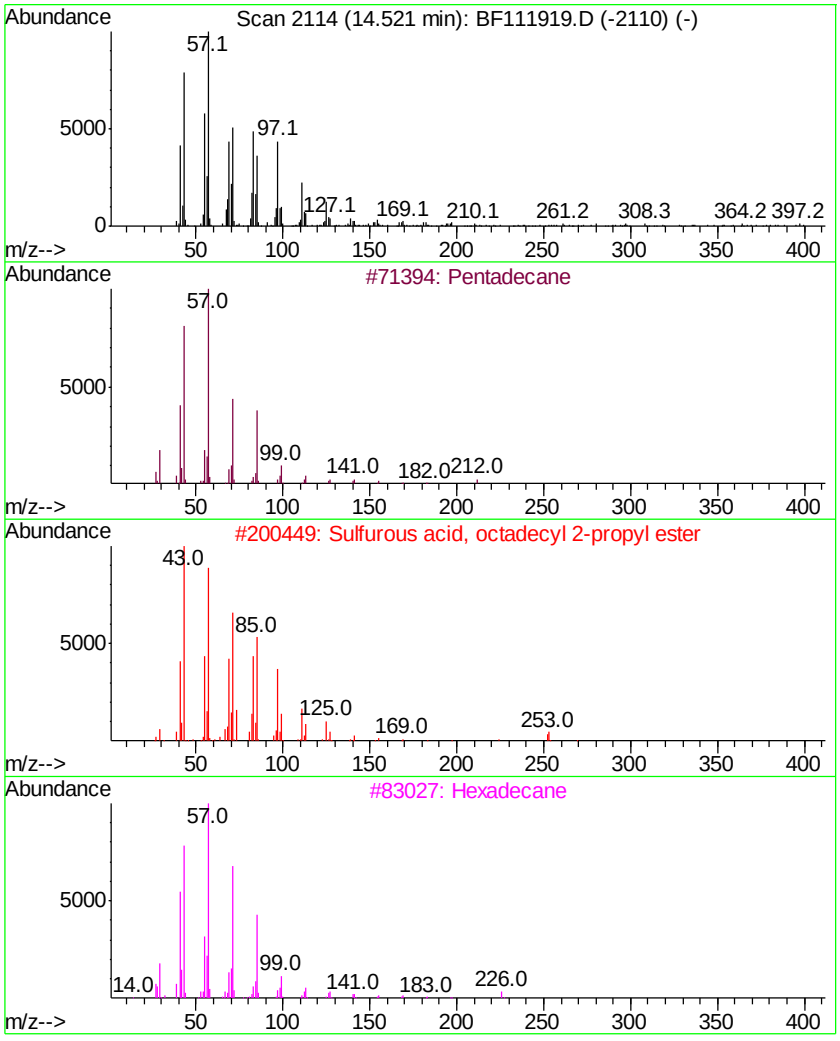
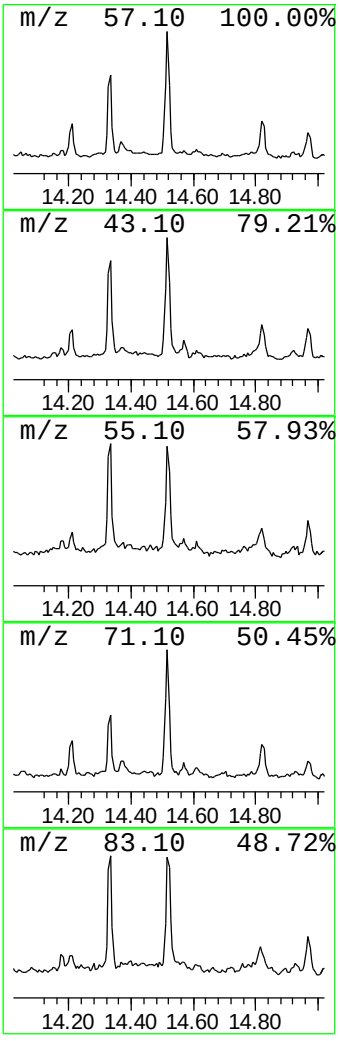
Peak Number 13 Pentadecane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.52 | 13.06 ng | 518629 | Chrysene-d12 | 14.05 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentadecane | 212 | C15H32 | 000629-62-9 | 92 |
| 2 | Sulfurous acid, octadecyl 2-prop... | 376 | C21H44O3S | 1000309-12-7 | 87 |
| 3 | Hexadecane | 226 | C16H34 | 000544-76-3 | 68 |
| 4 | Decane, 3,8-dimethyl- | 170 | C12H26 | 017312-55-9 | 62 |
| 5 | Dodecane, 2-methyl-6-propyl- | 226 | C16H34 | 055045-08-4 | 62 |



# Library Search Compound Report

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Data File : BF111919.D
Acq On : 8 Jan 2019 20:44
Operator : JU/SJ
Sample : K1044-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CPSB-08(20-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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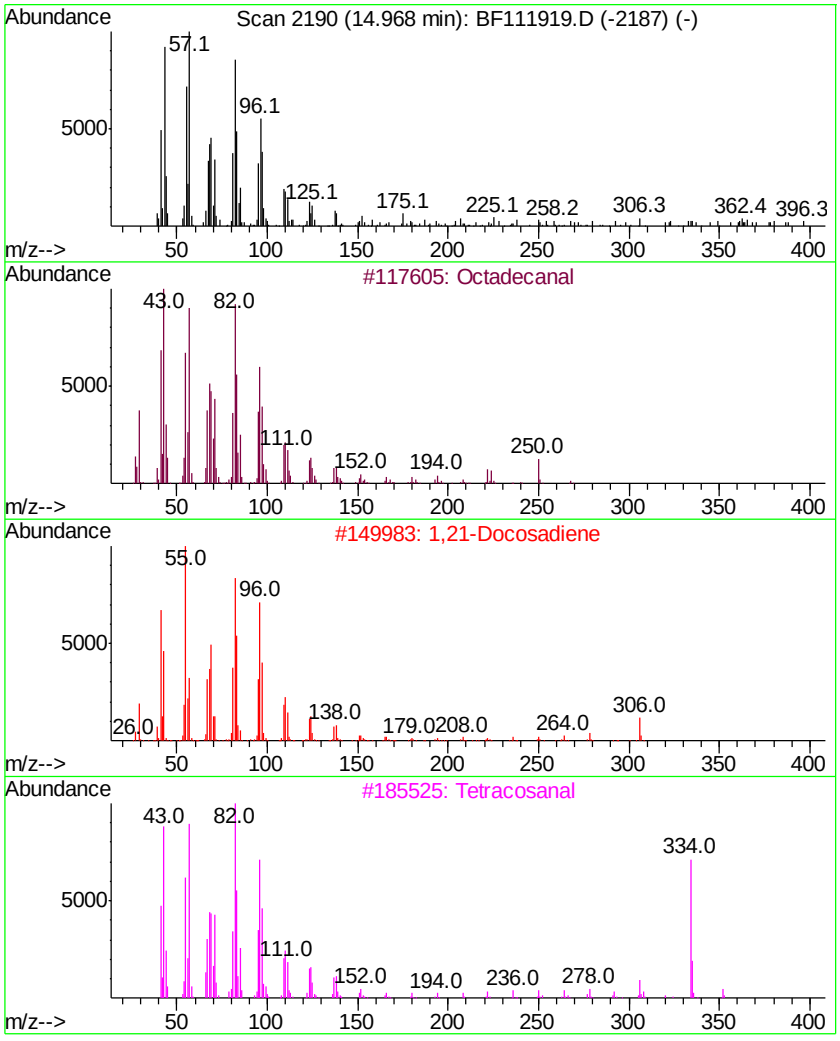
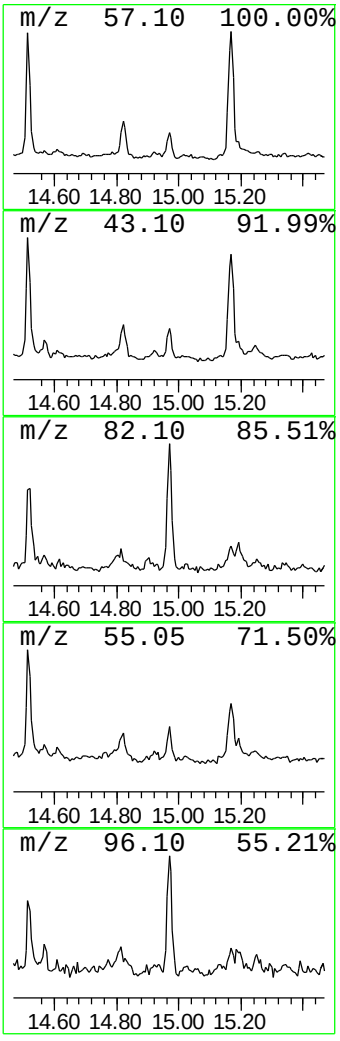
Peak Number 14 Octadecanal Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.97 | 5.27 ng | 221353 | Perylene-d12 | 15.53 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanal | 268 | C18H36O | 000638-66-4 | 96 |
| 2 | 1,21-Docosadiene | 306 | C22H42 | 053057-53-7 | 91 |
| 3 | Tetracosanal | 352 | C24H48O | 057866-08-7 | 91 |
| 4 | 17-Octadecenal | 266 | C18H34O | 056554-86-0 | 91 |
| 5 | 1,16-Hexadecanediol | 258 | C16H34O2 | 007735-42-4 | 90 |



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Data File : BF111919.D
Acq On : 8 Jan 2019 20:44
Operator : JU/SJ
Sample : K1044-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CPSB-08(20-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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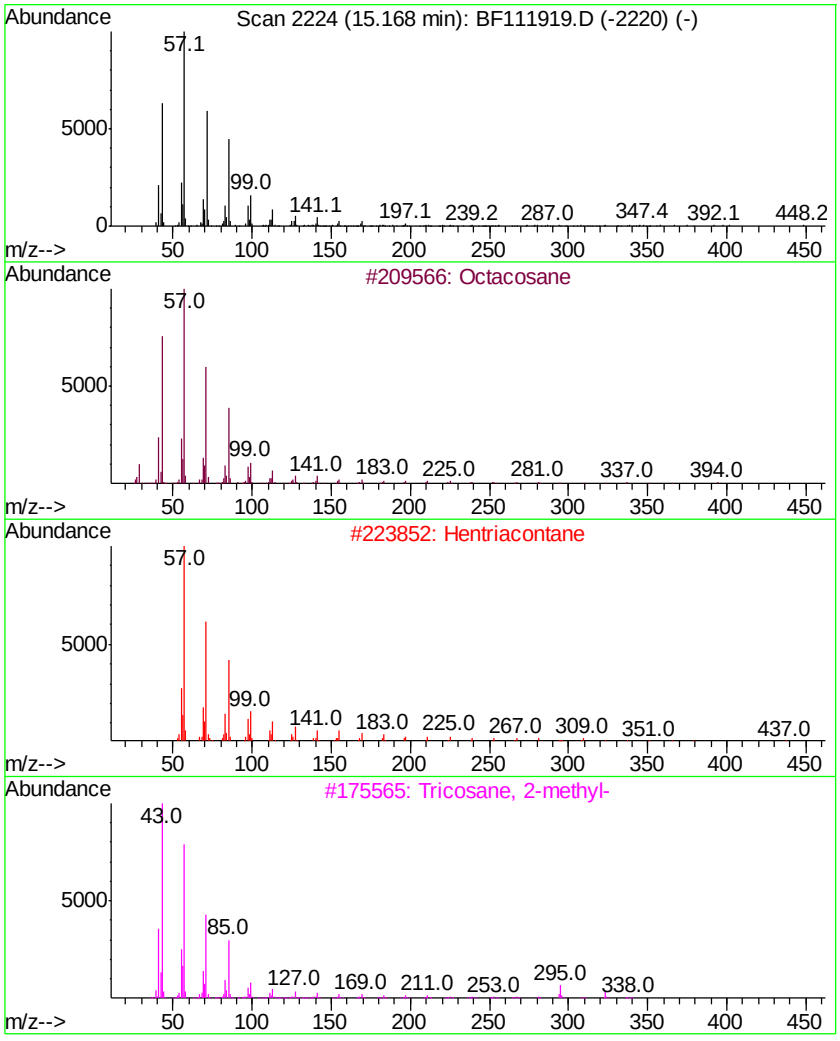
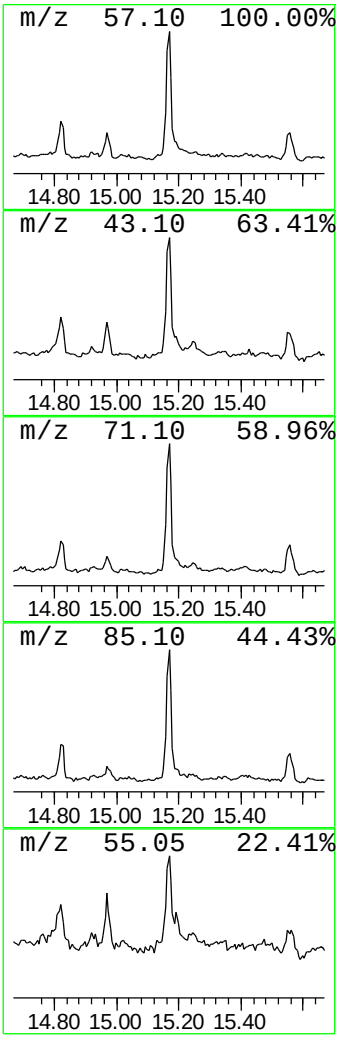
Peak Number 15 Octacosane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.17 | 11.48 ng | 482348 | Perylene-d12 | 15.53 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 2 | Hentriacontane | 437 | C31H64 | 000630-04-6 | 91 |
| 3 | Tricosane, 2-methyl- | 338 | C24H50 | 001928-30-9 | 90 |
| 4 | Tetracosane | 338 | C24H50 | 000646-31-1 | 90 |
| 5 | Docosane | 310 | C22H46 | 000629-97-0 | 87 |



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Data File : BF111919.D
Acq On : 8 Jan 2019 20:44
Operator : JU/SJ
Sample : K1044-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CPSB-08(20-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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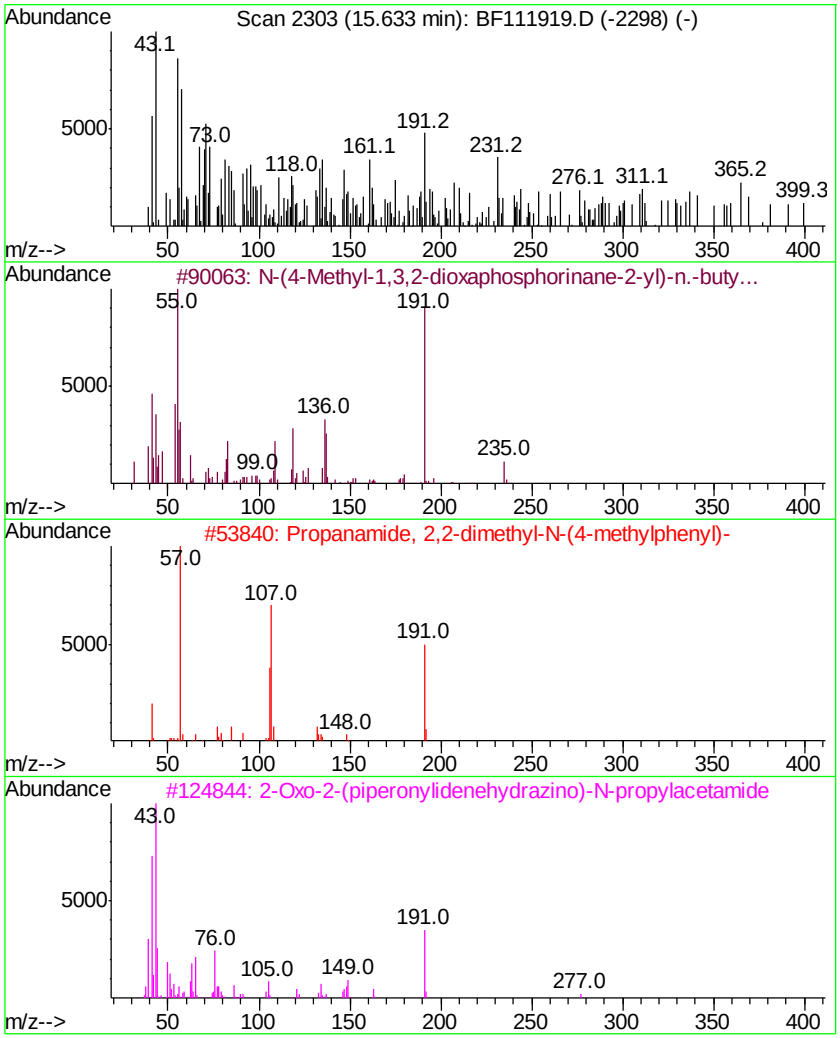
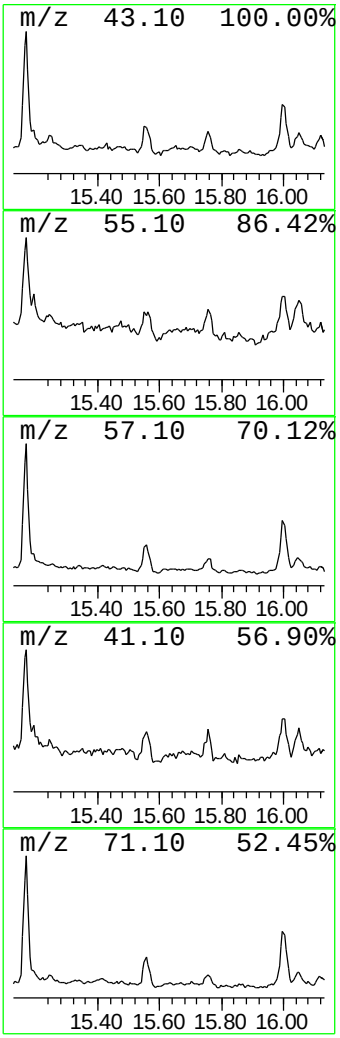
Peak Number 16 unknown15.63 Concentration Rank 19

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.63 | 2.74 ng | 115003 | Perylene-d12 | 15.53 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | N-(4-Methyl-1,3,2-dioxaphosphori... | 235 | C9H18NO4P | 1000140-31-5 | 10 |
| 2 | Propanamide, 2,2-dimethyl-N-(4-m... | 191 | C12H17NO | 021354-40-5 | 10 |
| 3 | 2-Oxo-2-(piperonylidenehydrazino... | 277 | C13H15N3O4 | 329713-81-7 | 10 |
| 4 | 4(1H)-Pteridinone, 2-amino-6,7-d... | 191 | C8H9N5O | 000611-55-2 | 9 |
| 5 | Tetradecanoic acid, (3,3a,4,6a,7... | 518 | C31H50O6 | 077573-28-5 | 9 |



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Operator : JU/SJ
Sample : K1044-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CPSB-08(20-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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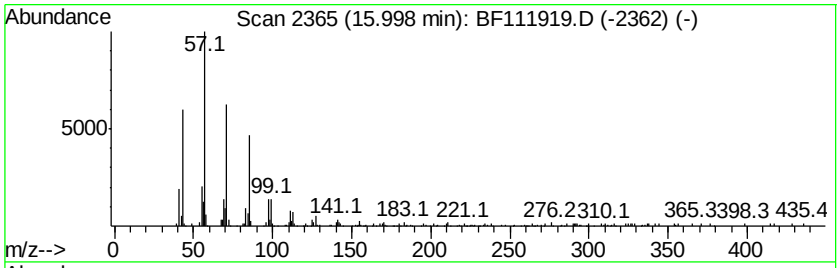
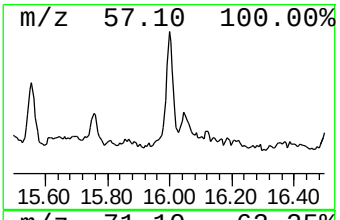
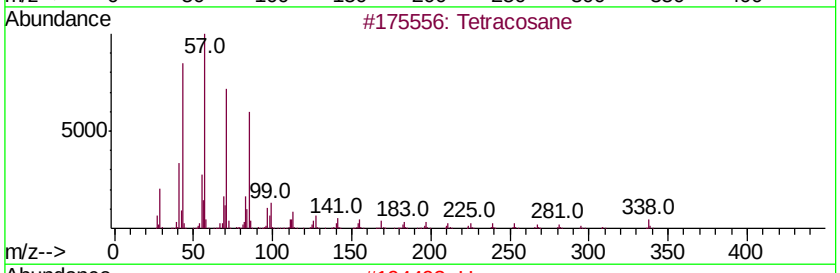
Peak Number 17 Tetracosane Concentration Rank 10

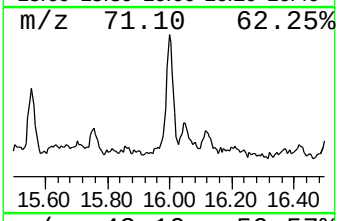
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.00 | 5.54 ng | 232812 | Perylene-d12 | 15.53 |

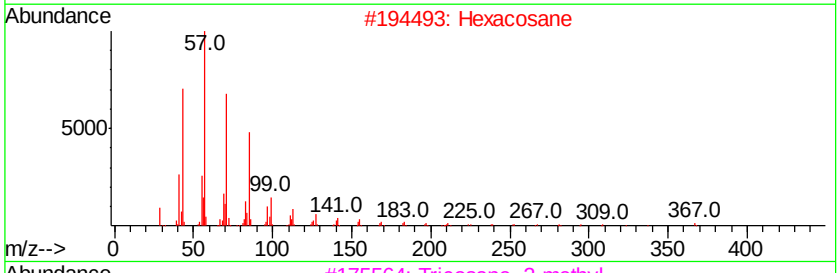
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetracosane | 338 | C24H50 | 000646-31-1 | 94 |
| 2 | Hexacosane | 366 | C26H54 | 000630-01-3 | 87 |
| 3 | Tricosane, 2-methyl- | 338 | C24H50 | 001928-30-9 | 86 |
| 4 | Nonadecane | 268 | C19H40 | 000629-92-5 | 80 |
| 5 | Heneicosane | 296 | C21H44 | 000629-94-7 | 74 |

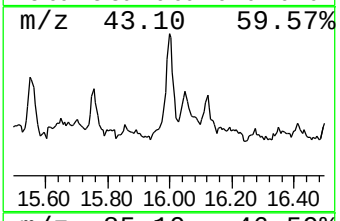


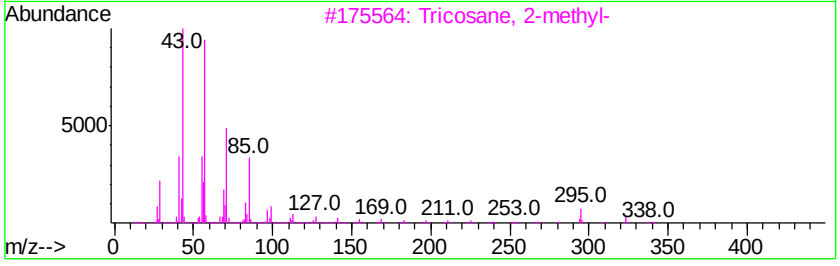



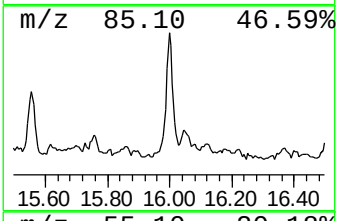



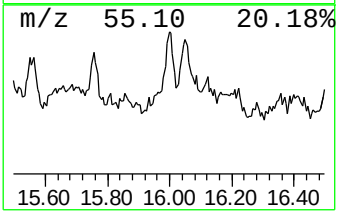



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010819\
Data File : BF111919.D
Acq On : 8 Jan 2019 20:44
Operator : JU/SJ
Sample : K1044-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CPSB-08(20-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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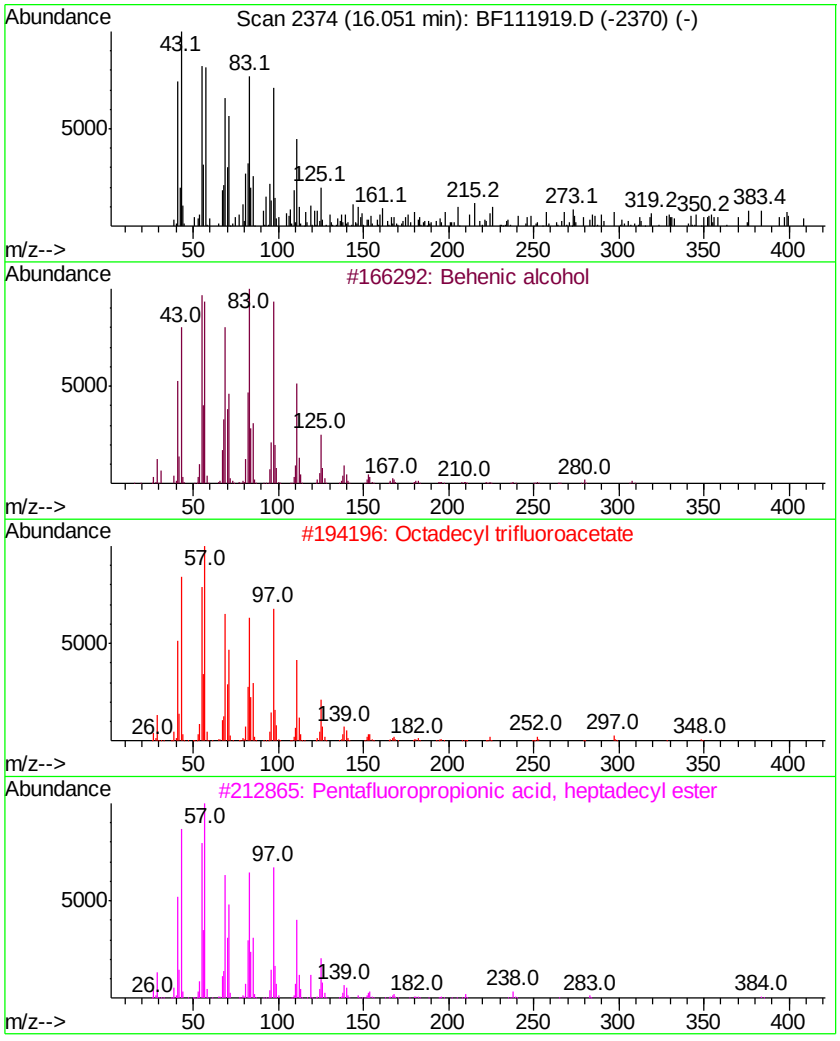
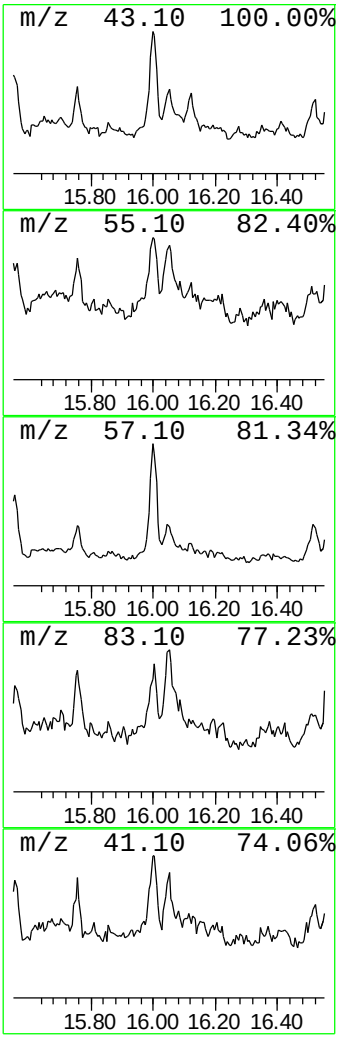
Peak Number 18 Behenic alcohol Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.05 | 4.14 ng | 173877 | Perylene-d12 | 15.53 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 93 |
| 2 | Octadecyl trifluoroacetate | 366 | C20H37F3O2 | 079392-43-1 | 93 |
| 3 | Pentafluoropropionic acid, hepta... | 402 | C20H35F5O2 | 959218-78-1 | 93 |
| 4 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 90 |
| 5 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 90 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010819\
Data File : BF111919.D
Acq On : 8 Jan 2019 20:44
Operator : JU/SJ
Sample : K1044-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CPSB-08(20-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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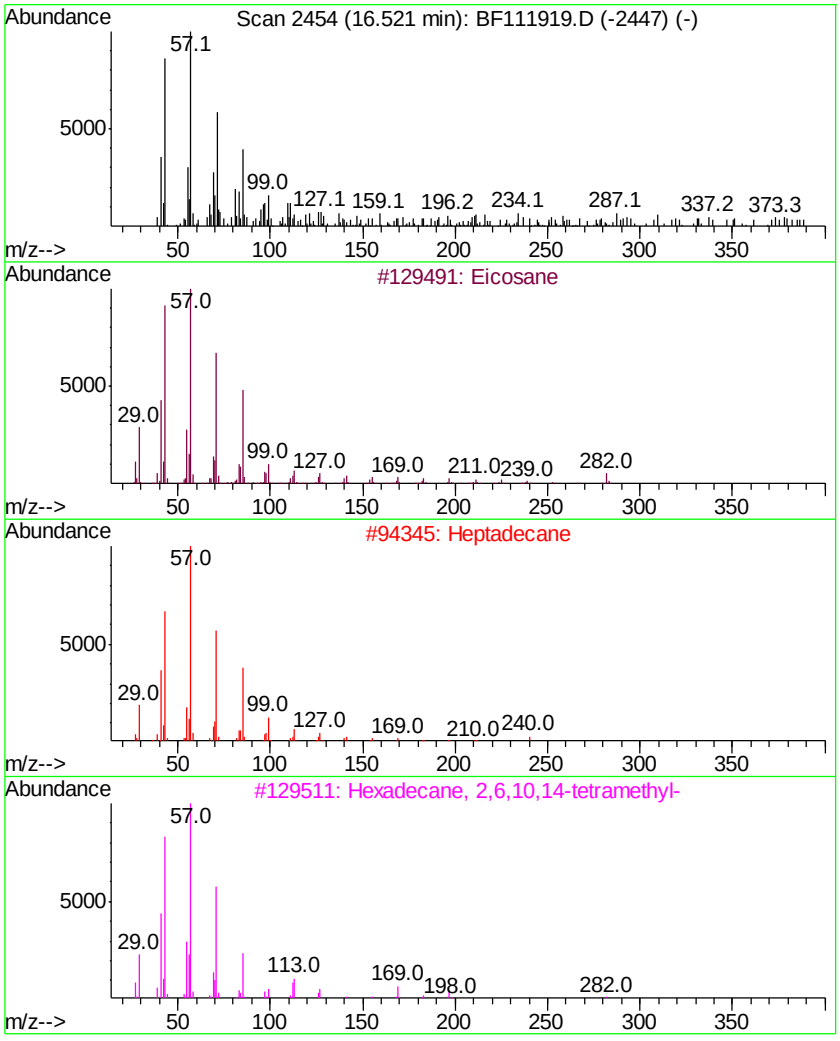
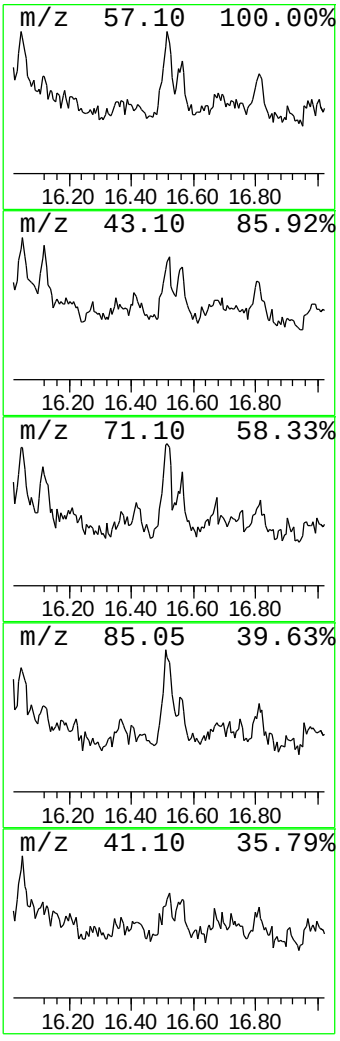
Peak Number 19 Eicosane Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.52 | 5.69 ng | 239123 | Perylene-d12 | 15.53 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Eicosane | 282 | C20H42 | 000112-95-8 | 78 |
| 2 | Heptadecane | 240 | C17H36 | 000629-78-7 | 78 |
| 3 | Hexadecane, 2,6,10,14-tetramethyl- | 282 | C20H42 | 000638-36-8 | 60 |
| 4 | Tetradecane, 4-methyl- | 212 | C15H32 | 025117-24-2 | 55 |
| 5 | Tetradecane | 198 | C14H30 | 000629-59-4 | 55 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010819\
Data File : BF111919.D
Acq On : 8 Jan 2019 20:44
Operator : JU/SJ
Sample : K1044-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CPSB-08(20-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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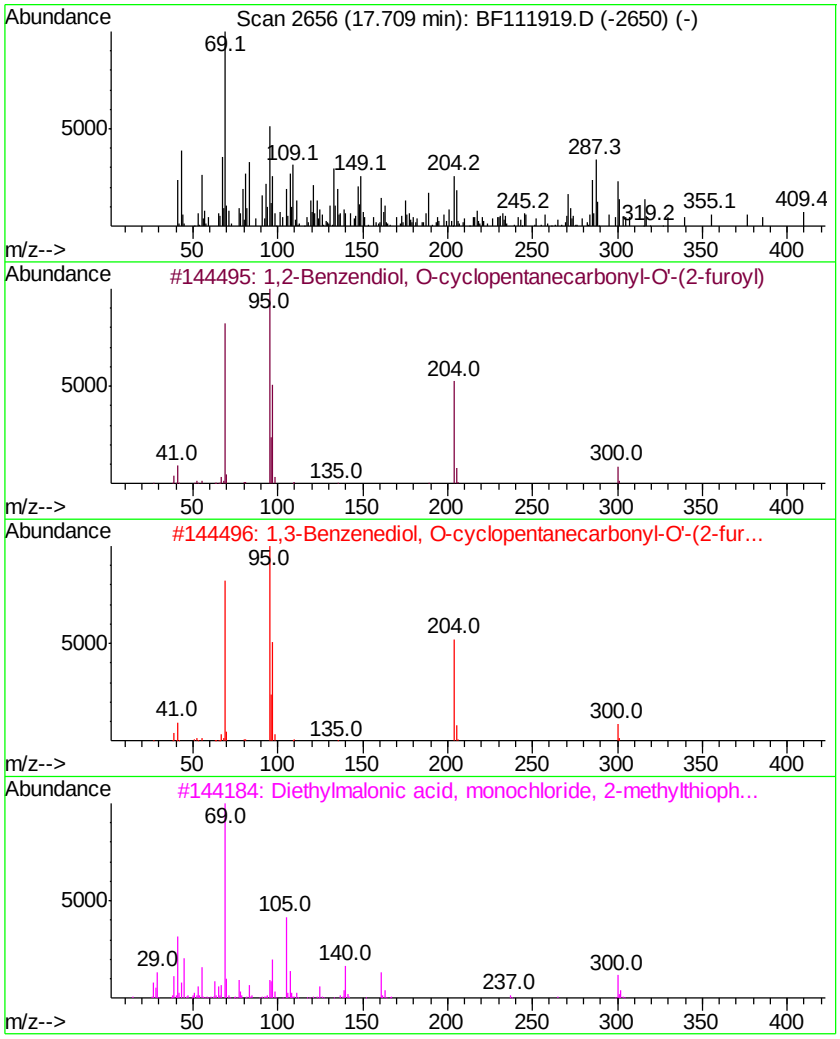
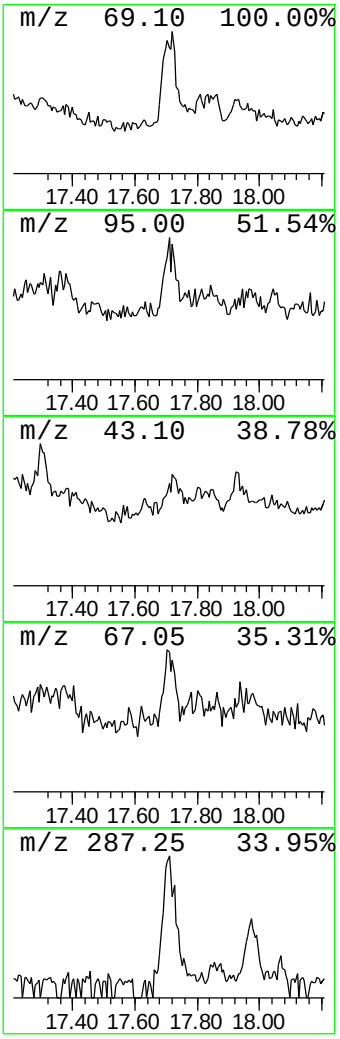
Peak Number 20 1,2-Benzendiol, O-cyclopent... Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.71 | 4.14 ng | 173883 | Perylene-d12 | 15.53 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,2-Benzendiol, O-cyclopentaneca... | 300 | C17H16O5 | 1000330-10-0 | 50 |
| 2 | 1,3-Benzenediol, O-cyclopentanec... | 300 | C17H16O5 | 1000345-56-4 | 50 |
| 3 | Diethylmalonic acid, monochlorid... | 300 | C14H17ClO3S | 1000369-54-4 | 43 |
| 4 | 2,6,10,14-Hexadecatetraene, 1-be... | 488 | C33H44OS | 1000194-30-4 | 27 |
| 5 | Aniline, N,N-di(trifluoroacetyl)- | 285 | C10H5F6NO2 | 1000328-30-7 | 25 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF010819\
Data File : BF111919.D
Acq On : 8 Jan 2019 20:44
Operator : JU/SJ
Sample : K1044-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** CPSB-08(20-25)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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 |
| Butane, 2-methoxy... | 2.20 | 3.3 | ng | 127405 | 1 | 6.89 | 782790 | 20.0 |
| 2-Pentanone, 4-hy... | 5.10 | 3.8 | ng | 149895 | 1 | 6.89 | 782790 | 20.0 |
| unknown6.66 | 6.66 | 62.8 | ng | 2458710 | 1 | 6.89 | 782790 | 20.0 |
| Heptadecane | 10.79 | 14.7 | ng | 523475 | 4 | 11.41 | 714538 | 20.0 |
| Heptadecane, 2,6,... | 11.30 | 2.7 | ng | 95562 | 4 | 11.41 | 714538 | 20.0 |
| n-Hexadecanoic acid | 11.93 | 4.1 | ng | 145689 | 4 | 11.41 | 714538 | 20.0 |
| 9,12-Octadecadien... | 12.48 | 3.0 | ng | 106864 | 4 | 11.41 | 714538 | 20.0 |
| 6-Octadecenoic ac... | 12.50 | 5.0 | ng | 177294 | 4 | 11.41 | 714538 | 20.0 |
| Bicyclo[10.8.0]ei... | 13.68 | 9.7 | ng | 384519 | 5 | 14.05 | 794442 | 20.0 |
| 5-Eicosene, (E)- | 13.89 | 14.4 | ng | 570908 | 5 | 14.05 | 794442 | 20.0 |
| Oxirane, hexadecyl- | 14.33 | 12.8 | ng | 508690 | 5 | 14.05 | 794442 | 20.0 |
| Pentadecane | 14.52 | 13.1 | ng | 518629 | 5 | 14.05 | 794442 | 20.0 |
| Octadecanal | 14.97 | 5.3 | ng | 221353 | 6 | 15.53 | 840019 | 20.0 |
| Octacosane | 15.17 | 11.5 | ng | 482348 | 6 | 15.53 | 840019 | 20.0 |
| unknown15.63 | 15.63 | 2.7 | ng | 115003 | 6 | 15.53 | 840019 | 20.0 |
| Tetracosane | 16.00 | 5.5 | ng | 232812 | 6 | 15.53 | 840019 | 20.0 |
| Behenic alcohol | 16.05 | 4.1 | ng | 173877 | 6 | 15.53 | 840019 | 20.0 |
| Eicosane | 16.52 | 5.7 | ng | 239123 | 6 | 15.53 | 840019 | 20.0 |
| 1,2-Benzendiol, O... | 17.71 | 4.1 | ng | 173883 | 6 | 15.53 | 840019 | 20.0 |