LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF021518\
Data File : BF103030.D
Acq On : 15 Feb 2018 20:59
Operator : SJ/JU
Sample : J1536-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMPOSITE-A-20180150

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-BF020318.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 | 2.157 | 6 | 12 | 19 | rVB | 959009 | 1217654 | 29.46% | 3.414% |
| 2 | 5.116 | 512 | 515 | 526 | rVB | 85095 | 113044 | 2.73% | 0.317% |
| 3 | 5.504 | 576 | 581 | 584 | rBV | 3835616 | 4011141 | 97.03% | 11.245% |
| 4 | 6.510 | 747 | 752 | 766 | rVB | 3545927 | 4133750 | 100.00% | 11.589% |
| 5 | 6.651 | 771 | 776 | 779 | rBV | 4068035 | 3915234 | 94.71% | 10.976% |
| 6 | 6.875 | 811 | 814 | 818 | rVB | 1182913 | 1048481 | 25.36% | 2.939% |
| 7 | 7.034 | 837 | 841 | 845 | rBV | 3247040 | 2945258 | 71.25% | 8.257% |
| 8 | 7.439 | 905 | 910 | 913 | rBV | 2365788 | 2386994 | 57.74% | 6.692% |
| 9 | 8.163 | 1029 | 1033 | 1038 | rBV | 1489926 | 1361497 | 32.94% | 3.817% |
| 10 | 9.233 | 1211 | 1215 | 1218 | rBV | 4037915 | 3606359 | 87.24% | 10.110% |
| 11 | 9.304 | 1224 | 1227 | 1230 | rVB | 95157 | 73995 | 1.79% | 0.207% |
| 12 | 9.622 | 1277 | 1281 | 1289 | rBV | 275356 | 292679 | 7.08% | 0.821% |
| 13 | 9.833 | 1314 | 1317 | 1322 | rBV | 179652 | 145362 | 3.52% | 0.408% |
| 14 | 9.916 | 1327 | 1331 | 1335 | rBV | 1633522 | 1404958 | 33.99% | 3.939% |
| 15 | 10.333 | 1400 | 1402 | 1405 | rVB | 202319 | 155866 | 3.77% | 0.437% |
| 16 | 10.557 | 1433 | 1440 | 1442 | rBV | 54628 | 70935 | 1.72% | 0.199% |
| 17 | 10.704 | 1462 | 1465 | 1472 | rBV | 1879986 | 1806540 | 43.70% | 5.065% |
| 18 | 10.810 | 1479 | 1483 | 1493 | rVB | 188981 | 216784 | 5.24% | 0.608% |
| 19 | 11.257 | 1556 | 1559 | 1561 | rBV | 120455 | 96693 | 2.34% | 0.271% |
| 20 | 11.286 | 1561 | 1564 | 1569 | rVB2 | 43821 | 47272 | 1.14% | 0.133% |
| 21 | 11.404 | 1580 | 1584 | 1588 | rBV | 1361668 | 1154106 | 27.92% | 3.236% |
| 22 | 11.616 | 1616 | 1620 | 1629 | rBV2 | 46803 | 48573 | 1.18% | 0.136% |
| 23 | 12.169 | 1711 | 1714 | 1717 | rVB | 125393 | 93113 | 2.25% | 0.261% |
| 24 | 12.798 | 1818 | 1821 | 1824 | rBV | 55437 | 46362 | 1.12% | 0.130% |
| 25 | 12.986 | 1849 | 1853 | 1857 | rBV | 2546660 | 2407507 | 58.24% | 6.749% |
| 26 | 13.868 | 2000 | 2003 | 2012 | rVB | 504055 | 482691 | 11.68% | 1.353% |
| 27 | 14.045 | 2029 | 2033 | 2037 | rBV | 996997 | 918666 | 22.22% | 2.575% |
| 28 | 14.168 | 2052 | 2054 | 2057 | rVV | 37685 | 43961 | 1.06% | 0.123% |
| 29 | 14.210 | 2059 | 2061 | 2064 | rVB | 56854 | 52109 | 1.26% | 0.146% |
| 30 | 14.504 | 2108 | 2111 | 2115 | rBV5 | 44067 | 53709 | 1.30% | 0.151% |
| 31 | 14.880 | 2171 | 2175 | 2179 | rBV | 587960 | 563976 | 13.64% | 1.581% |
| 32 | 15.527 | 2281 | 2285 | 2292 | rBV | 561254 | 754536 | 18.25% | 2.115% |

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF021518\
Data File : BF103030.D
Acq On : 15 Feb 2018 20:59
Operator : SJ/JU
Sample : J1536-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
COMPOSITE-A-20180150

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-BF020318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

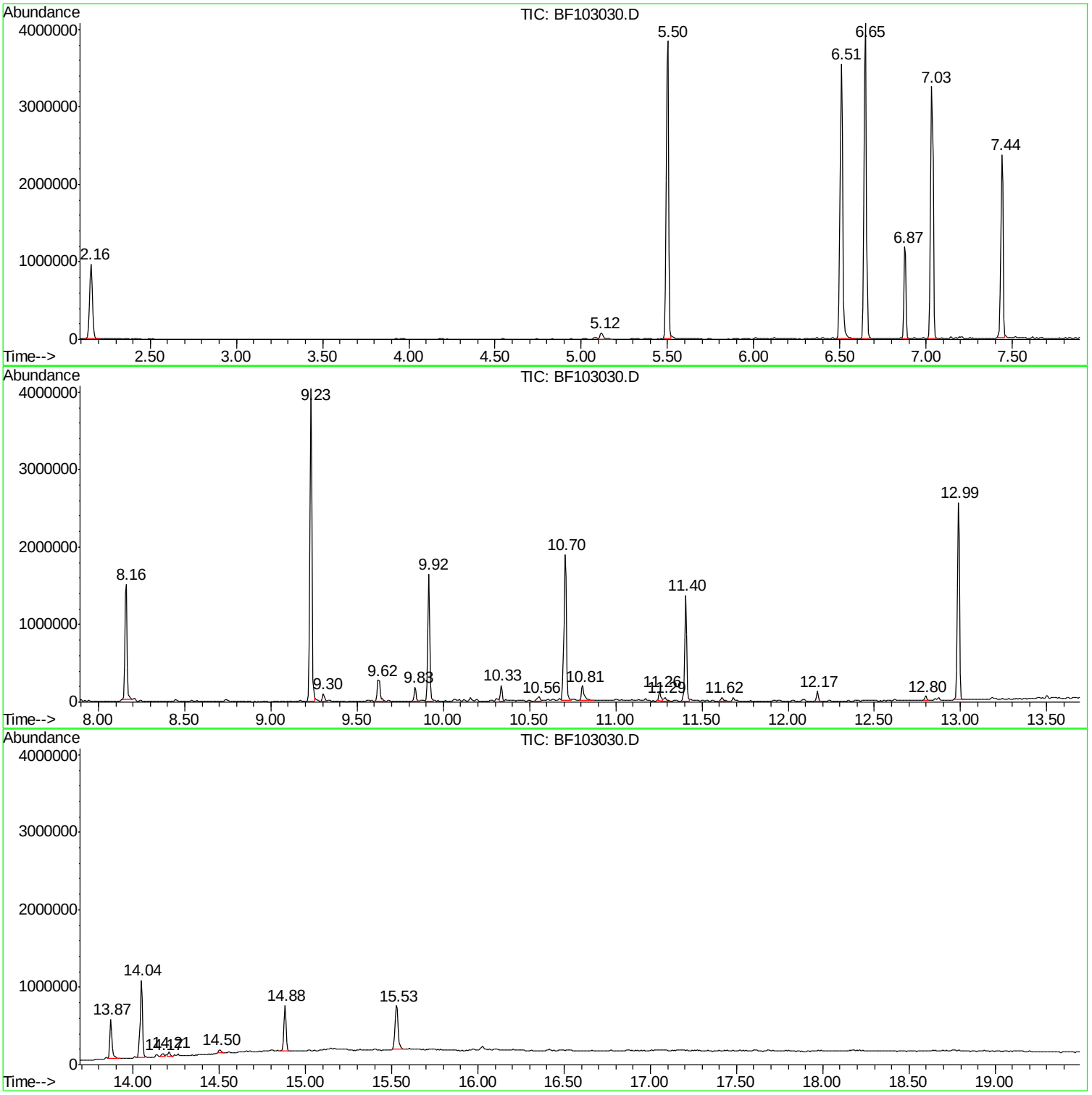
Sum of corrected areas: 35669805

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF021518\
Data File : BF103030.D
Acq On : 15 Feb 2018 20:59
Operator : SJ/JU
Sample : J1536-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
COMPOSITE-A-20180150

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF021518\
Data File : BF103030.D
Acq On : 15 Feb 2018 20:59
Operator : SJ/JU
Sample : J1536-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
COMPOSITE-A-20180150

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

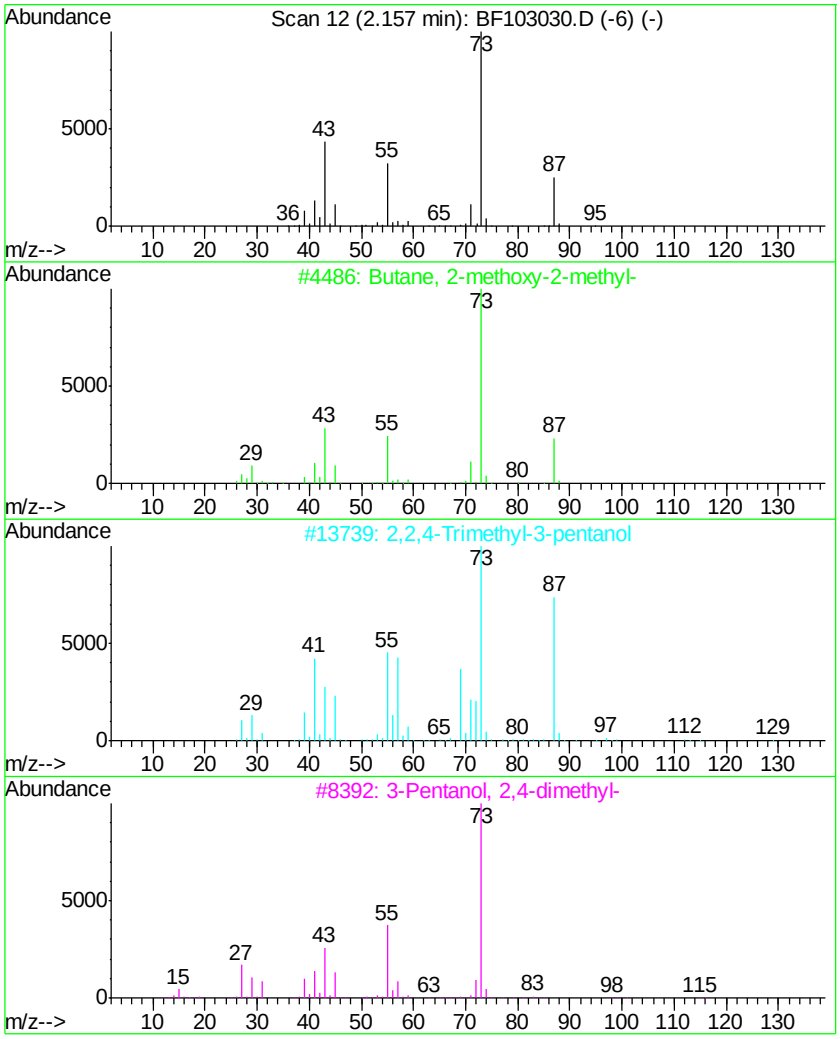
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

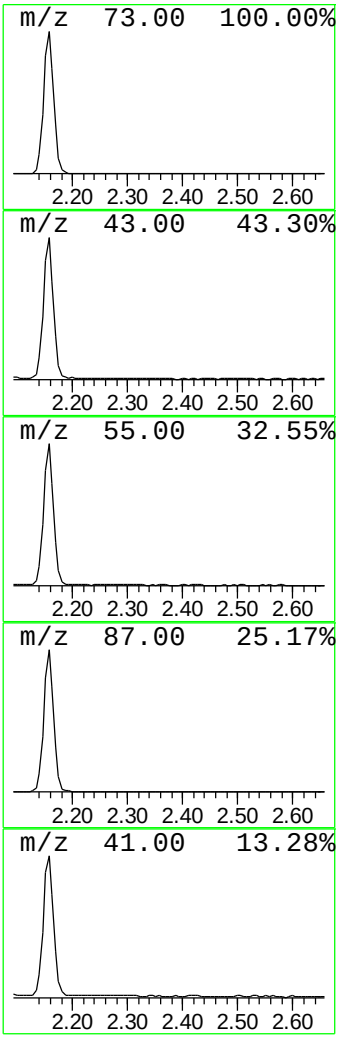
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.16 | 23.23 ng | 1217650 | 1,4-Dichlorobenzene-d4 | 6.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 83 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 39 |
| 3 | 3-Pentanol, 2,4-dimethyl- | 116 | C7H16O | 000600-36-2 | 37 |
| 4 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 35 |
| 5 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 25 |



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF021518\
Data File : BF103030.D
Acq On : 15 Feb 2018 20:59
Operator : SJ/JU
Sample : J1536-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
COMPOSITE-A-20180150

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

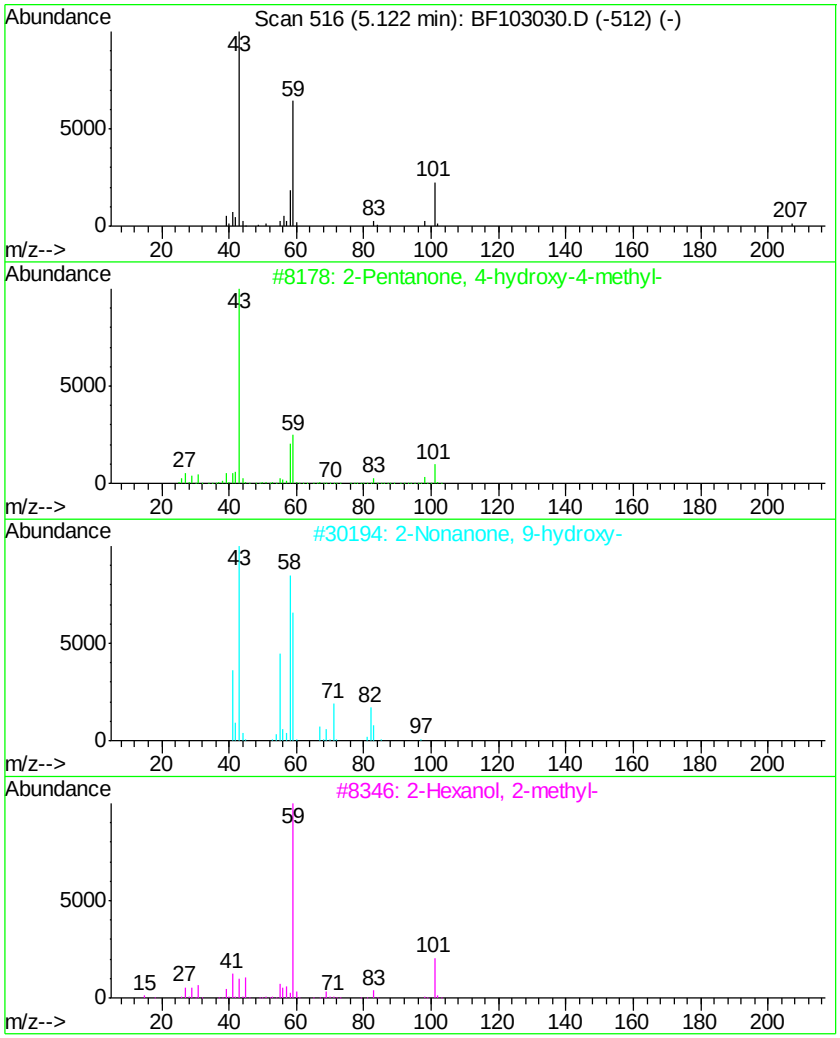
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

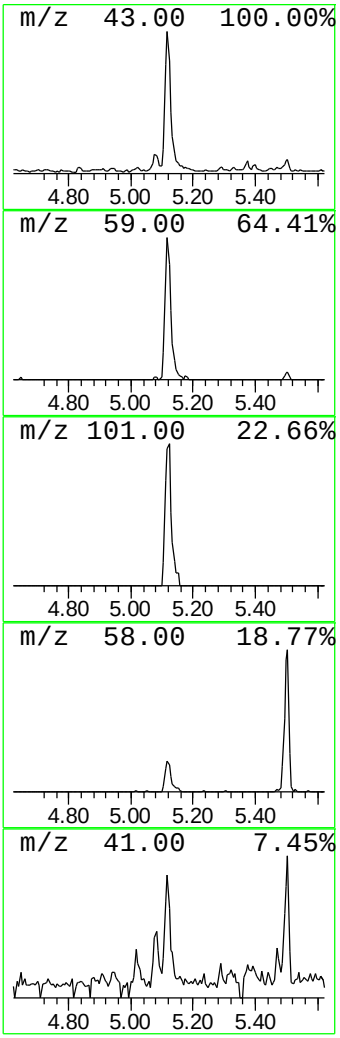
**********

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.12 | 2.16 ng | 113044 | 1,4-Dichlorobenzene-d4 | 6.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 53 |
| 2 | 2-Nonanone, 9-hydroxy- | 158 | C9H18O2 | 025368-56-3 | 36 |
| 3 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 28 |
| 4 | Acetone | 58 | C3H6O | 000067-64-1 | 22 |
| 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\BF021518\
Data File : BF103030.D
Acq On : 15 Feb 2018 20:59
Operator : SJ/JU
Sample : J1536-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMPOSITE-A-20180150

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

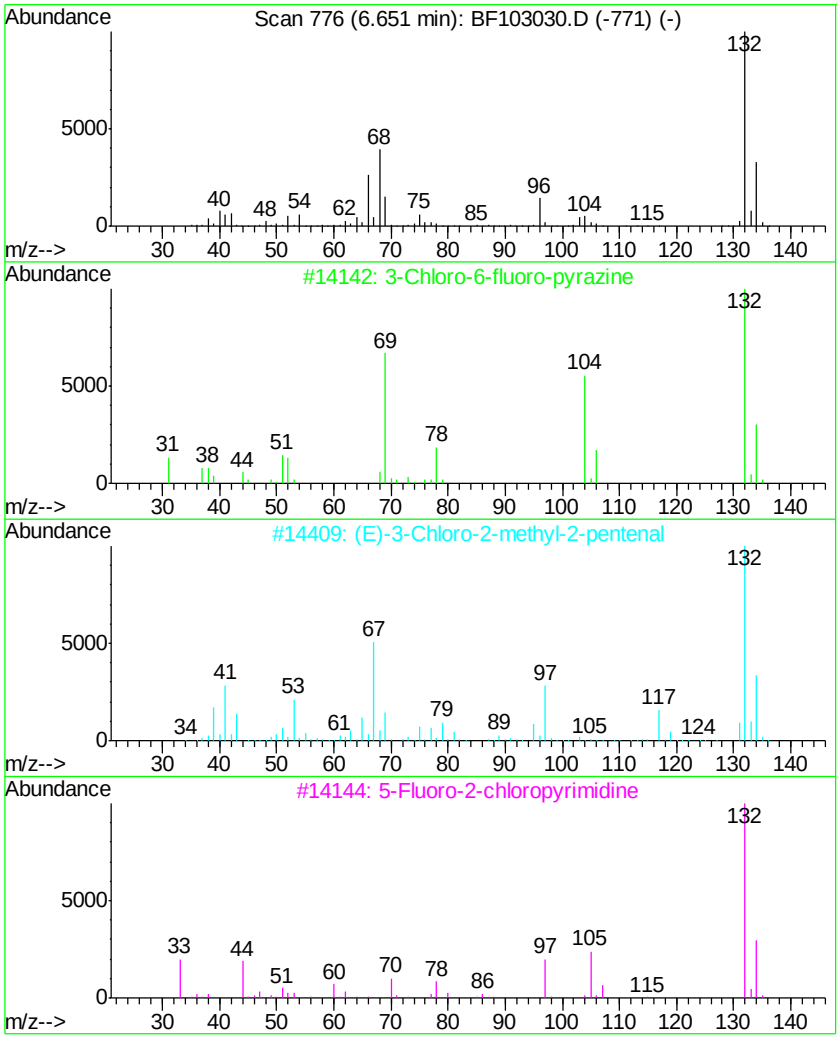
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

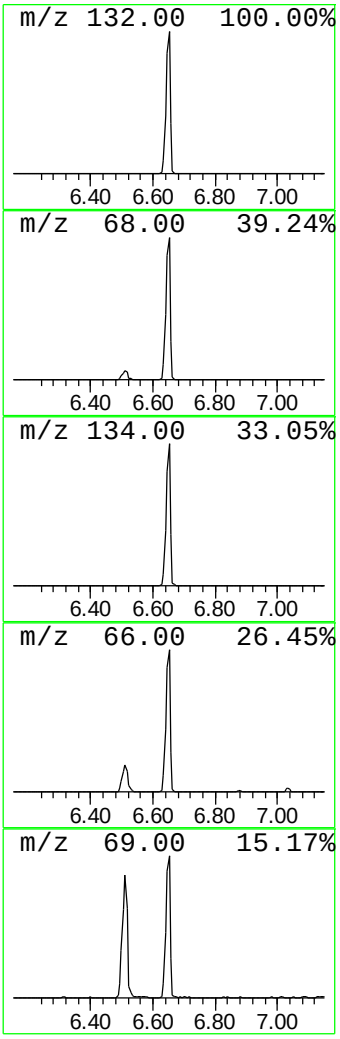
**********

Peak Number 3 unknown6.65 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.65 | 74.68 ng | 3915230 | 1,4-Dichlorobenzene-d4 | 6.87 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 16 |
| 3 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 4 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 5 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF021518\
Data File : BF103030.D
Acq On : 15 Feb 2018 20:59
Operator : SJ/JU
Sample : J1536-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
COMPOSITE-A-20180150

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

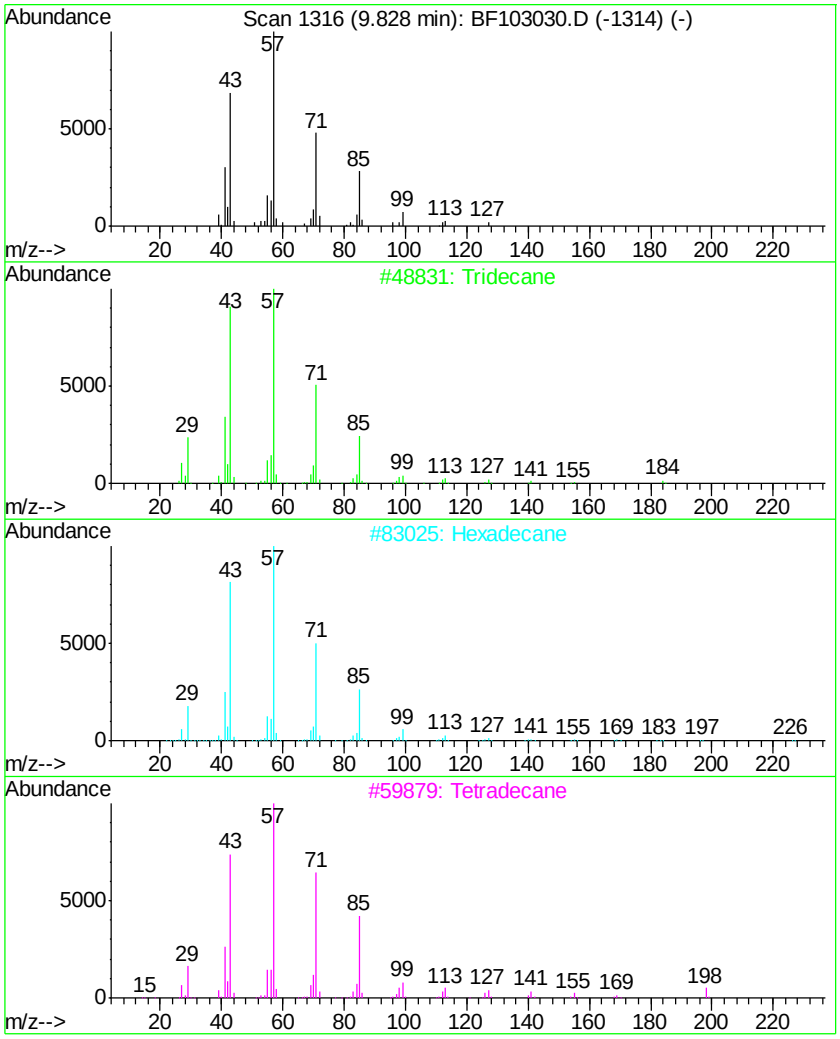
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

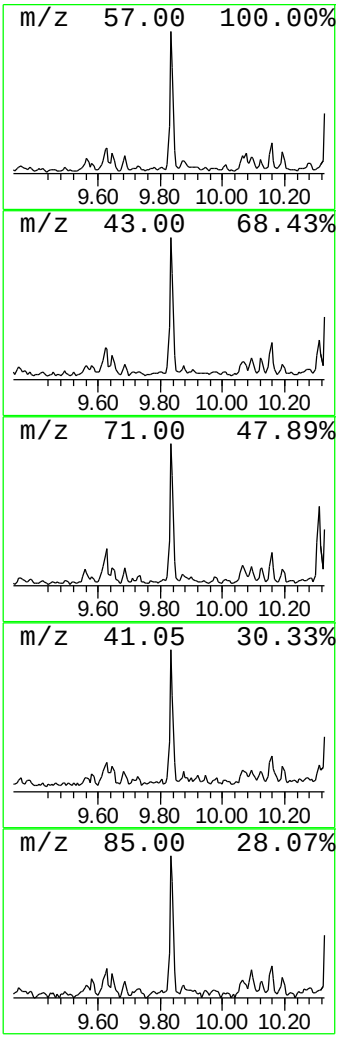
**********

Peak Number 5 Tridecane Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.83 | 2.07 ng | 145362 | Acenaphthene-d10 | 9.92 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tridecane | 184 | C13H28 | 000629-50-5 | 90 |
| 2 | Hexadecane | 226 | C16H34 | 000544-76-3 | 90 |
| 3 | Tetradecane | 198 | C14H30 | 000629-59-4 | 86 |
| 4 | Sulfurous acid, 2-ethylhexyl hex... | 278 | C14H30O3S | 1000309-20-2 | 80 |
| 5 | Decane, 2,9-dimethyl- | 170 | C12H26 | 001002-17-1 | 64 |



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF021518\
Data File : BF103030.D
Acq On : 15 Feb 2018 20:59
Operator : SJ/JU
Sample : J1536-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMPOSITE-A-20180150

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

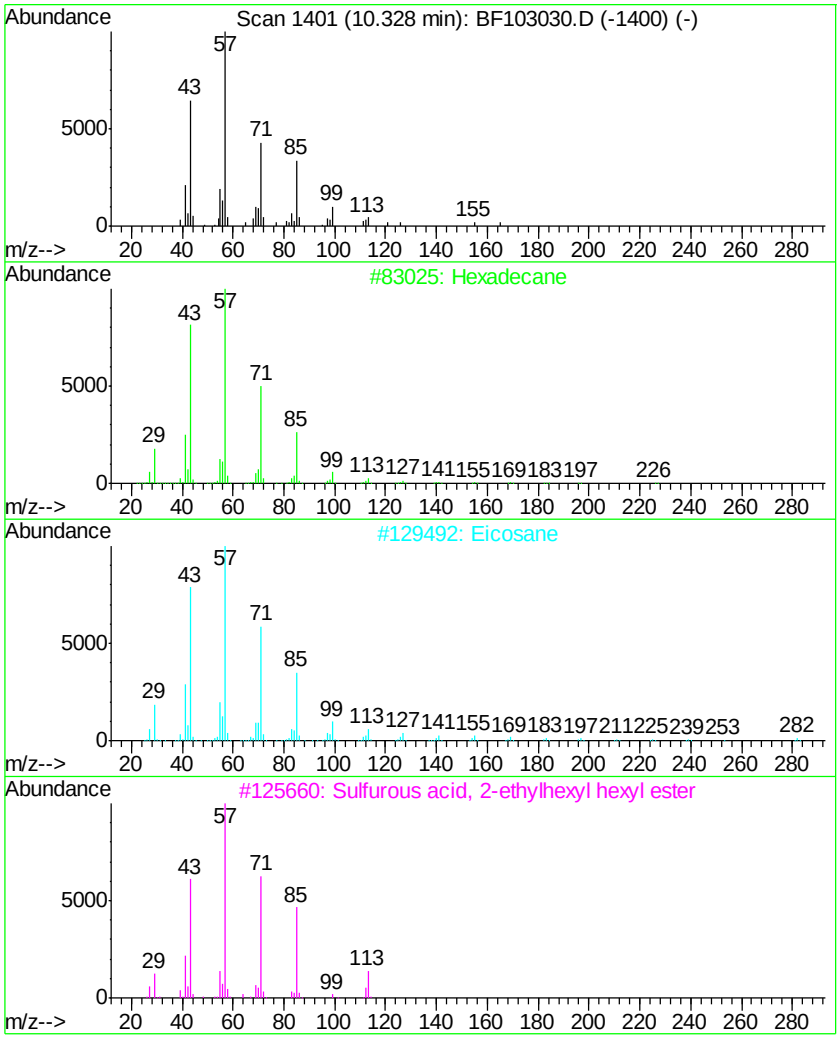
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

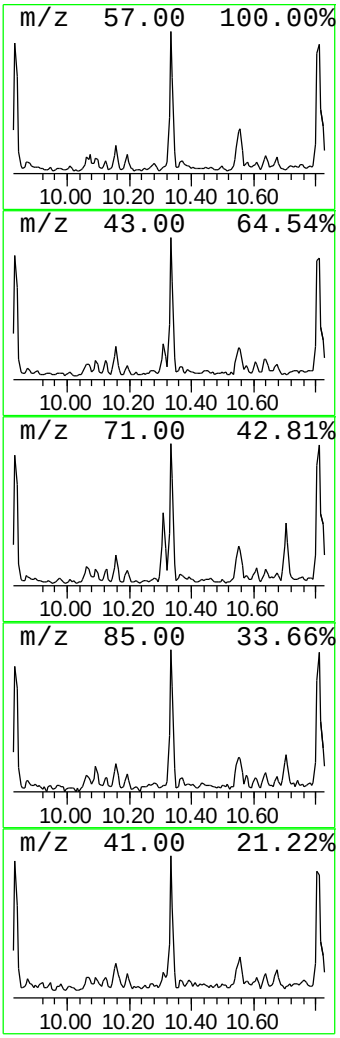
**********

Peak Number 6 Hexadecane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.33 | 2.22 ng | 155866 | Acenaphthene-d10 | 9.92 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane | 226 | C16H34 | 000544-76-3 | 78 |
| 2 | Eicosane | 282 | C20H42 | 000112-95-8 | 72 |
| 3 | Sulfurous acid, 2-ethylhexyl hex... | 278 | C14H30O3S | 1000309-20-2 | 64 |
| 4 | Undecane, 2-methyl- | 170 | C12H26 | 007045-71-8 | 64 |
| 5 | Sulfurous acid, decyl 2-propyl e... | 264 | C13H28O3S | 1000309-12-1 | 59 |



# Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF021518\
Data File : BF103030.D
Acq On : 15 Feb 2018 20:59
Operator : SJ/JU
Sample : J1536-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMPOSITE-A-20180150

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

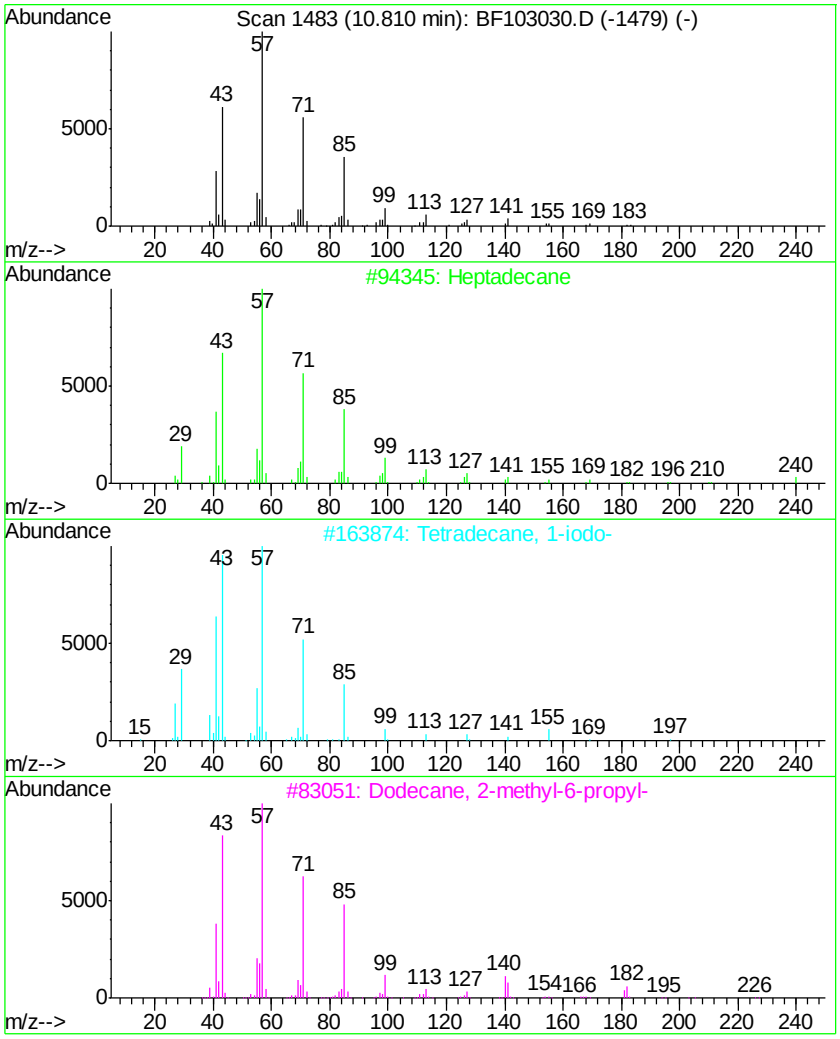
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

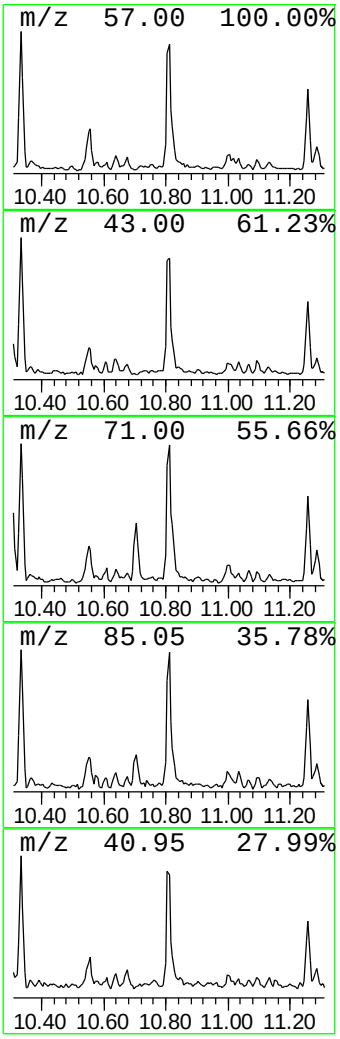
**********

Peak Number 7 Heptadecane Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.81 | 3.76 ng | 216784 | Phenanthrene-d10 | 11.40 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heptadecane | 240 | C17H36 | 000629-78-7 | 90 |
| 2 | Tetradecane, 1-iodo- | 324 | C14H29I | 019218-94-1 | 86 |
| 3 | Dodecane, 2-methyl-6-propyl- | 226 | C16H34 | 055045-08-4 | 86 |
| 4 | Hexadecane | 226 | C16H34 | 000544-76-3 | 78 |
| 5 | Heptacosane | 380 | C27H56 | 000593-49-7 | 72 |



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF021518\
Data File : BF103030.D
Acq On : 15 Feb 2018 20:59
Operator : SJ/JU
Sample : J1536-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMPOSITE-A-20180150

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

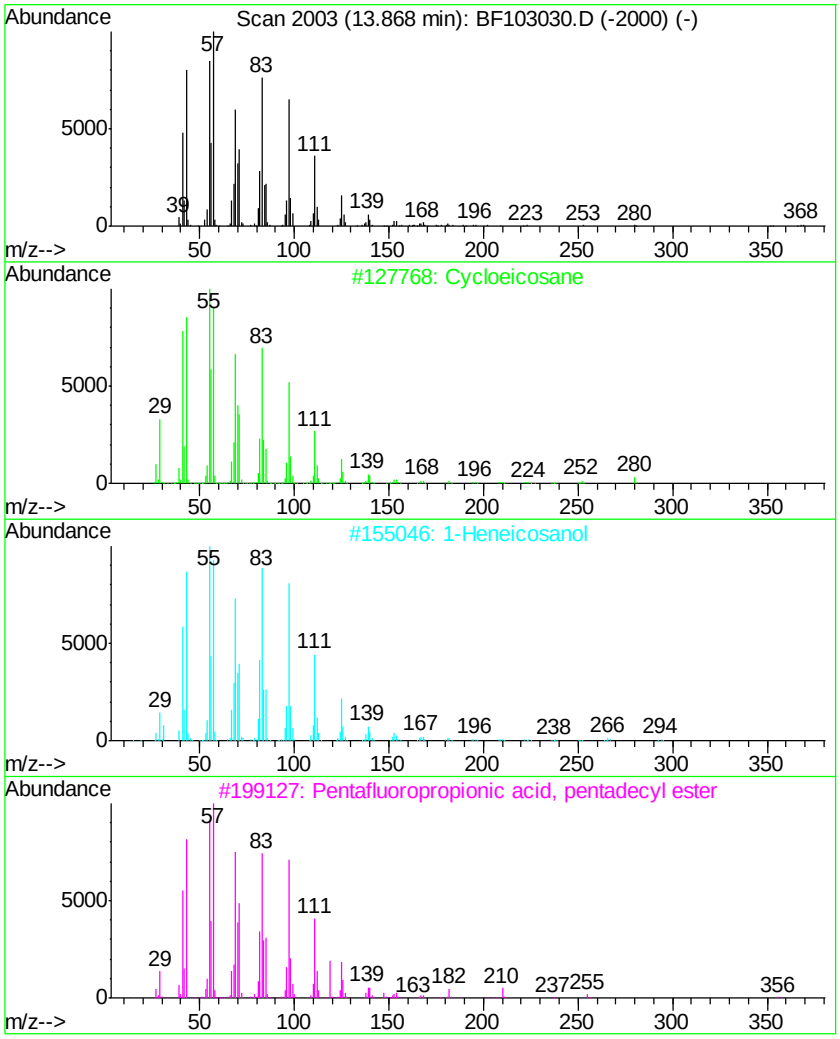
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

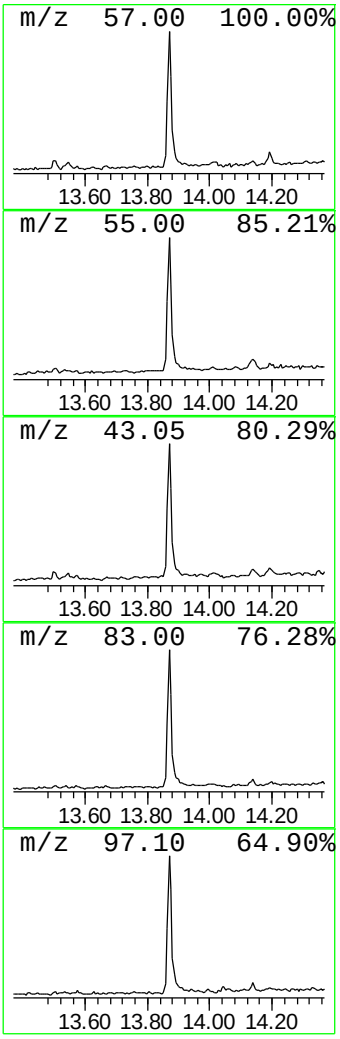
**********

Peak Number 8 Cycloeicosane Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.87 | 10.51 ng | 482691 | Chrysene-d12 | 14.04 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cycloeicosane | 280 | C20H40 | 000296-56-0 | 97 |
| 2 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 95 |
| 3 | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1 | 94 |
| 4 | Cyclotetradecane | 196 | C14H28 | 000295-17-0 | 93 |
| 5 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 93 |



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF021518\
Data File : BF103030.D
Acq On : 15 Feb 2018 20:59
Operator : SJ/JU
Sample : J1536-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMPOSITE-A-20180150

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

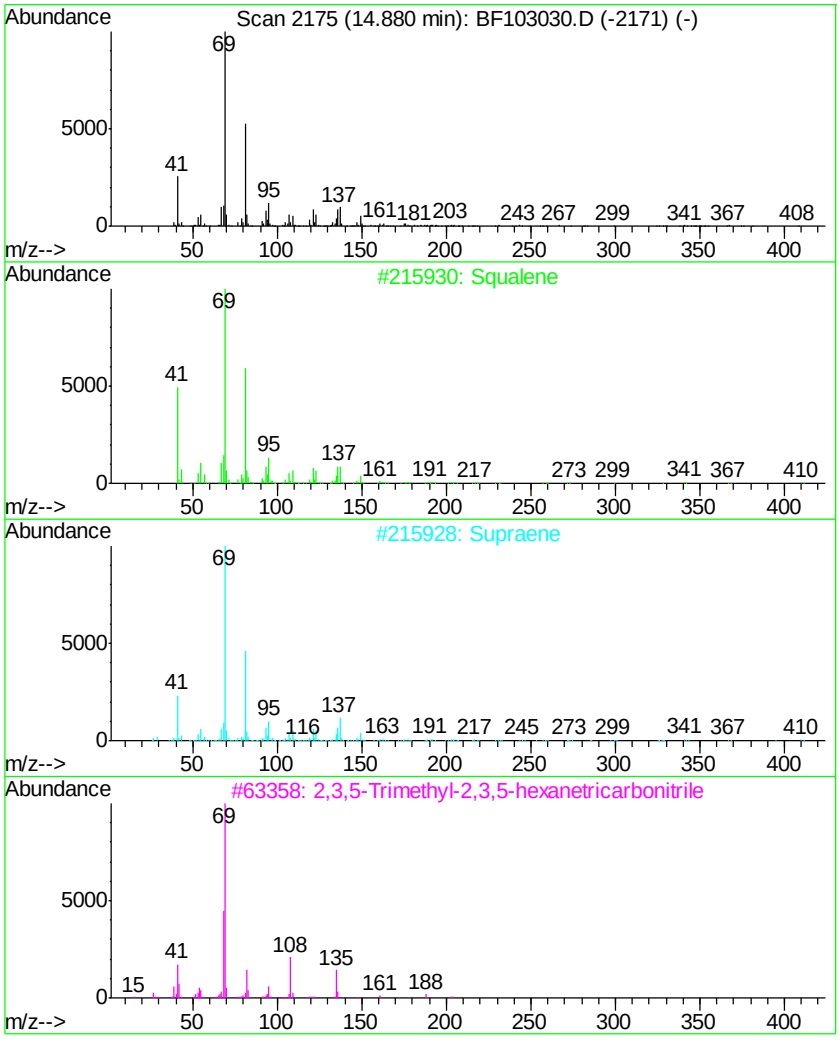
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

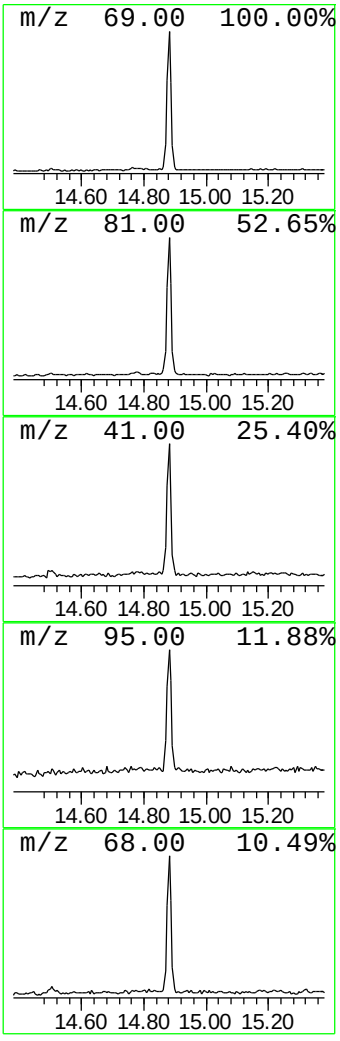
**********

Peak Number 9 Squalene Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.88 | 14.95 ng | 563976 | Perylene-d12 | 15.53 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Squalene | 410 | C30H50 | 000111-02-4 | 91 |
| 2 | Supraene | 410 | C30H50 | 007683-64-9 | 87 |
| 3 | 2,3,5-Trimethyl-2,3,5-hexanetric... | 203 | C12H17N3 | 003974-79-6 | 59 |
| 4 | 1,5-Heptadiene, 3,3,6-trimethyl- | 138 | C10H18 | 035387-63-4 | 58 |
| 5 | 1,5-Heptadiene, 3,3-dimethyl-, (E)- | 124 | C9H16 | 067682-47-7 | 50 |



Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF021518\
Data File : BF103030.D
Acq On : 15 Feb 2018 20:59
Operator : SJ/JU
Sample : J1536-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** COMPOSITE-A-20180150

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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... | 2.16 | 23.2 | ng | 1217650 | 1 | 6.87 | 1048480 | 20.0 |
| 2-Pentanone, 4-hy... | 5.12 | 2.2 | ng | 113044 | 1 | 6.87 | 1048480 | 20.0 |
| unknown6.65 | 6.65 | 74.7 | ng | 3915230 | 1 | 6.87 | 1048480 | 20.0 |
| Tridecane | 9.83 | 2.1 | ng | 145362 | 3 | 9.92 | 1404960 | 20.0 |
| Hexadecane | 10.33 | 2.2 | ng | 155866 | 3 | 9.92 | 1404960 | 20.0 |
| Heptadecane | 10.81 | 3.8 | ng | 216784 | 4 | 11.40 | 1154110 | 20.0 |
| Cycloeicosane | 13.87 | 10.5 | ng | 482691 | 5 | 14.04 | 918666 | 20.0 |
| Squalene | 14.88 | 14.9 | ng | 563976 | 6 | 15.53 | 754536 | 20.0 |