LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020718\
Data File : BF102841.D
Acq On : 8 Feb 2018 3:31
Operator : SJ/JU
Sample : J1458-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-02

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 | 2.181 | 8 | 16 | 24 | rVB | 422279 | 562890 | 12.48% | 1.540% |
| 2 | 5.122 | 513 | 516 | 523 | rVB | 116903 | 145091 | 3.22% | 0.397% |
| 3 | 5.504 | 576 | 581 | 584 | rBV | 4365217 | 4509793 | 100.00% | 12.341% |
| 4 | 6.510 | 747 | 752 | 772 | rBV | 3781174 | 4447703 | 98.62% | 12.171% |
| 5 | 6.657 | 772 | 777 | 780 | rVV | 4136685 | 4333056 | 96.08% | 11.857% |
| 6 | 6.716 | 783 | 787 | 790 | rVB | 55611 | 46974 | 1.04% | 0.129% |
| 7 | 6.880 | 812 | 815 | 819 | rVB | 1081653 | 975952 | 21.64% | 2.671% |
| 8 | 7.039 | 838 | 842 | 846 | rBV | 3600844 | 3330940 | 73.86% | 9.115% |
| 9 | 7.445 | 906 | 911 | 914 | rBV | 2802018 | 2786581 | 61.79% | 7.626% |
| 10 | 7.475 | 914 | 916 | 920 | rVB | 54756 | 47900 | 1.06% | 0.131% |
| 11 | 8.163 | 1030 | 1033 | 1037 | rVB | 1292480 | 1187955 | 26.34% | 3.251% |
| 12 | 9.239 | 1211 | 1216 | 1226 | rBV | 4075272 | 3933658 | 87.22% | 10.764% |
| 13 | 9.316 | 1226 | 1229 | 1231 | rVB | 90920 | 71776 | 1.59% | 0.196% |
| 14 | 9.627 | 1279 | 1282 | 1286 | rBV | 388108 | 390760 | 8.66% | 1.069% |
| 15 | 9.845 | 1312 | 1319 | 1322 | rBV | 206209 | 167575 | 3.72% | 0.459% |
| 16 | 9.921 | 1328 | 1332 | 1341 | rVB | 1303630 | 1142443 | 25.33% | 3.126% |
| 17 | 10.345 | 1397 | 1404 | 1407 | rBV2 | 216597 | 204244 | 4.53% | 0.559% |
| 18 | 10.563 | 1436 | 1441 | 1444 | rBV | 51362 | 66283 | 1.47% | 0.181% |
| 19 | 10.710 | 1462 | 1466 | 1476 | rVB | 2066509 | 2016837 | 44.72% | 5.519% |
| 20 | 10.816 | 1482 | 1484 | 1494 | rVB | 152753 | 165145 | 3.66% | 0.452% |
| 21 | 11.268 | 1557 | 1561 | 1563 | rBV | 56787 | 47520 | 1.05% | 0.130% |
| 22 | 11.410 | 1581 | 1585 | 1589 | rBV | 1097916 | 927799 | 20.57% | 2.539% |
| 23 | 11.927 | 1669 | 1673 | 1681 | rBV2 | 157540 | 168217 | 3.73% | 0.460% |
| 24 | 12.992 | 1850 | 1854 | 1858 | rBV | 2776829 | 2691077 | 59.67% | 7.364% |
| 25 | 13.880 | 2001 | 2005 | 2009 | rBV | 430377 | 444228 | 9.85% | 1.216% |
| 26 | 14.051 | 2030 | 2034 | 2040 | rVB | 922028 | 882794 | 19.58% | 2.416% |
| 27 | 14.145 | 2047 | 2050 | 2054 | rBV5 | 43136 | 46904 | 1.04% | 0.128% |
| 28 | 14.815 | 2161 | 2164 | 2168 | rVB2 | 46177 | 52936 | 1.17% | 0.145% |
| 29 | 14.892 | 2174 | 2177 | 2182 | rVB | 43818 | 52487 | 1.16% | 0.144% |
| 30 | 15.533 | 2281 | 2286 | 2296 | rBV | 475178 | 695408 | 15.42% | 1.903% |

Sum of corrected areas: 36542926

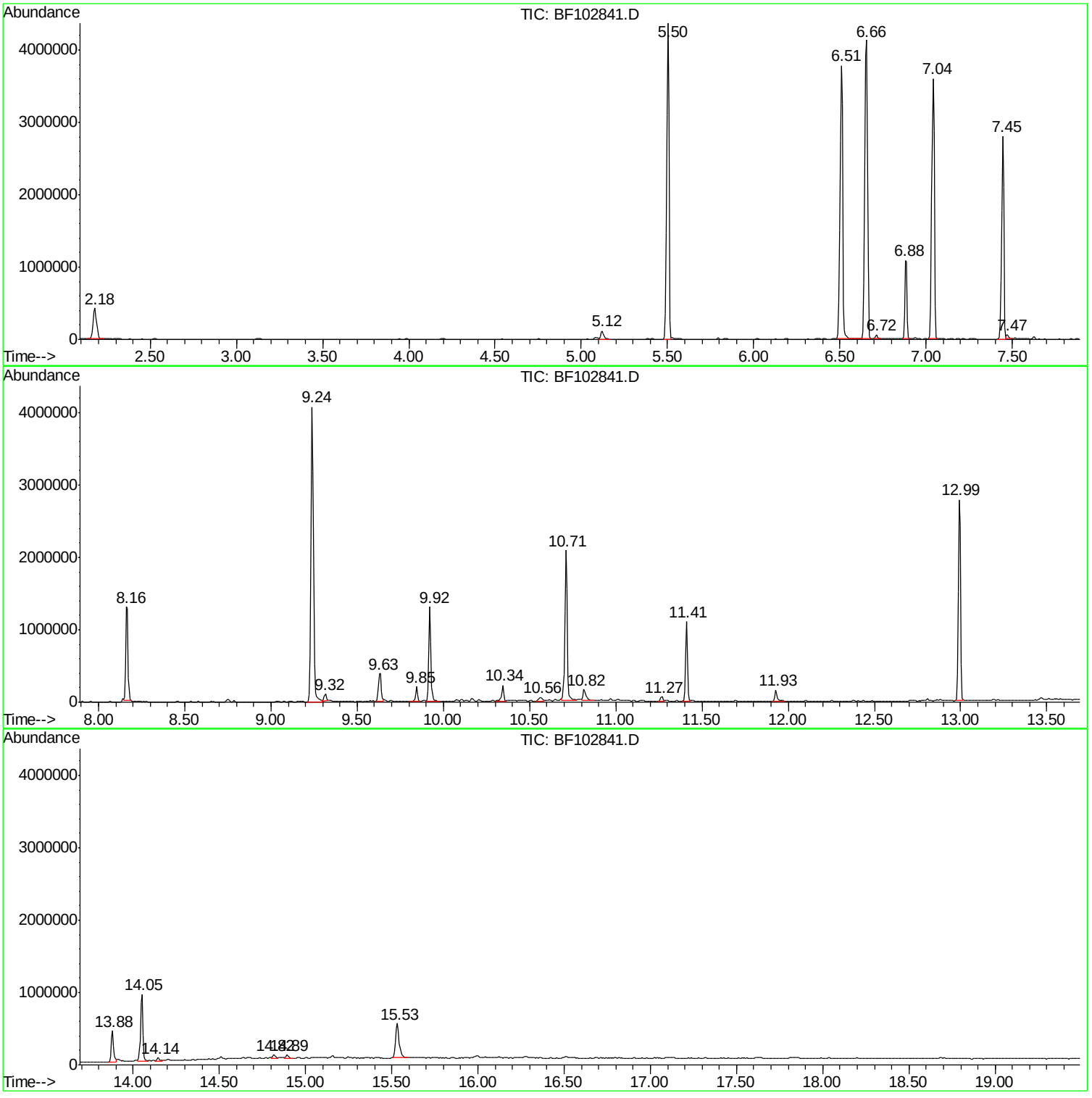
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020718\
Data File : BF102841.D
Acq On : 8 Feb 2018 3:31
Operator : SJ/JU
Sample : J1458-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-02

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 : Z:\HPCHEM1\BNA F\DATA\BF020718\
Data File : BF102841.D
Acq On : 8 Feb 2018 3:31
Operator : SJ/JU
Sample : J1458-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-02

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

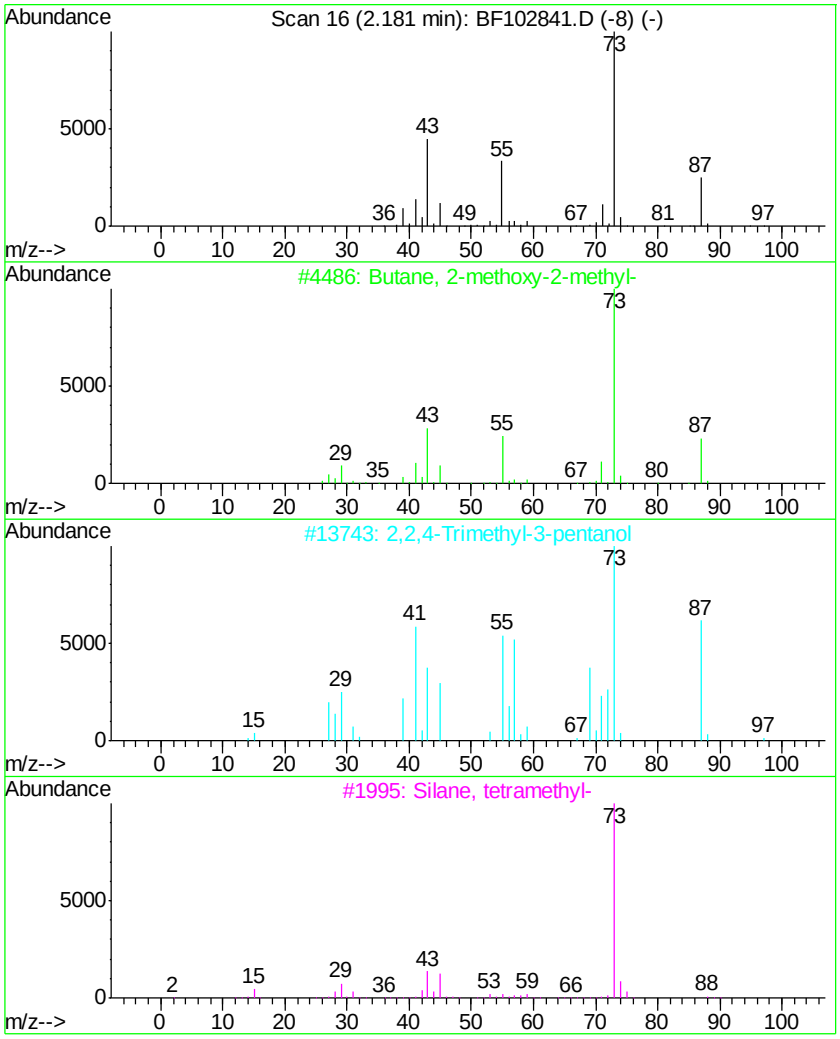
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

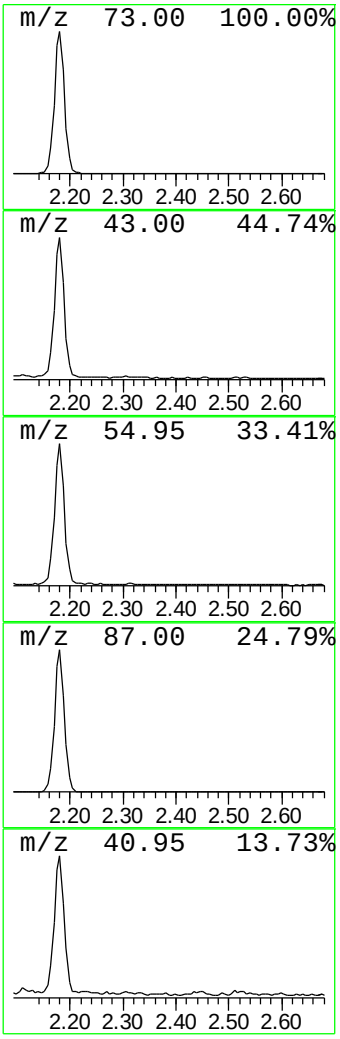
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.18 | 11.54 ng | 562890 | 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 | 83 |
| 2 | 2,2,4-Trimethyl-3-pentanol | 130 | C8H18O | 005162-48-1 | 39 |
| 3 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 35 |
| 4 | 2-Methyl-5-hexen-3-ol | 114 | C7H14O | 032815-70-6 | 28 |
| 5 | 2-Hydroxy-2-methylbutyric acid | 118 | C5H10O3 | 003739-30-8 | 25 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020718\
Data File : BF102841.D
Acq On : 8 Feb 2018 3:31
Operator : SJ/JU
Sample : J1458-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-02

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

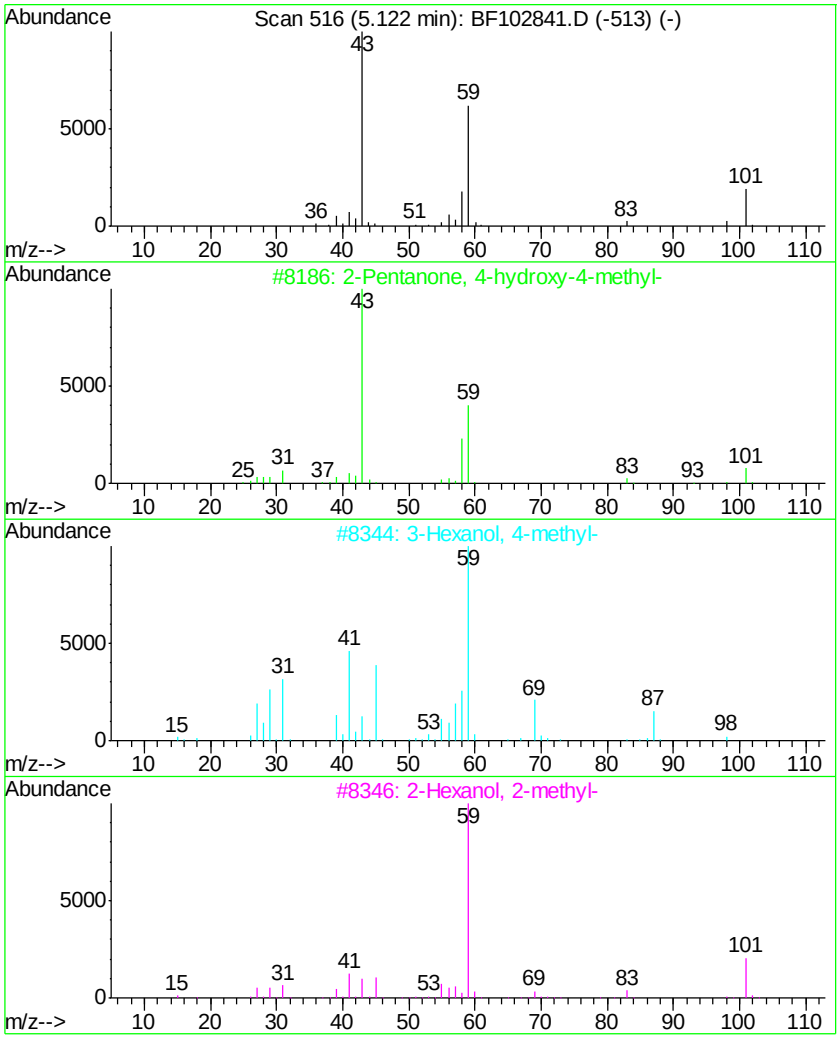
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

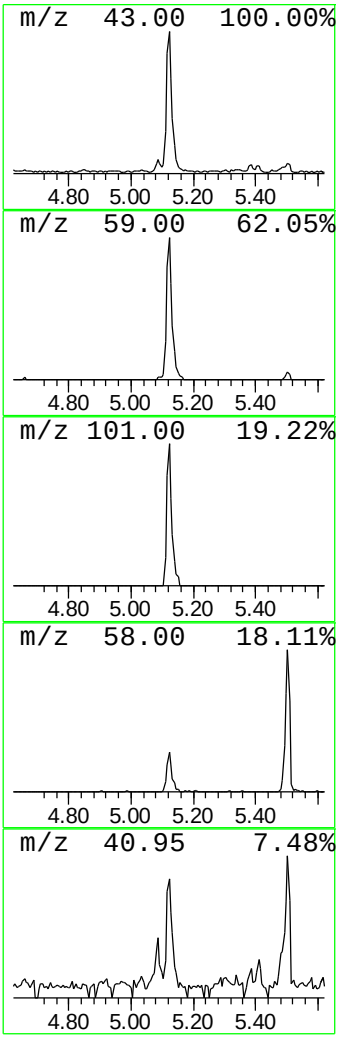
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.12 | 2.97 ng | 145091 | 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 | 72 |
| 2 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 28 |
| 3 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 28 |
| 4 | 1,2-Butanediol | 90 | C4H10O2 | 000584-03-2 | 23 |
| 5 | 3-Hydroxy-3-methyl-2-butanone | 102 | C5H10O2 | 000115-22-0 | 12 |



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020718\
Data File : BF102841.D
Acq On : 8 Feb 2018 3:31
Operator : SJ/JU
Sample : J1458-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-02

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

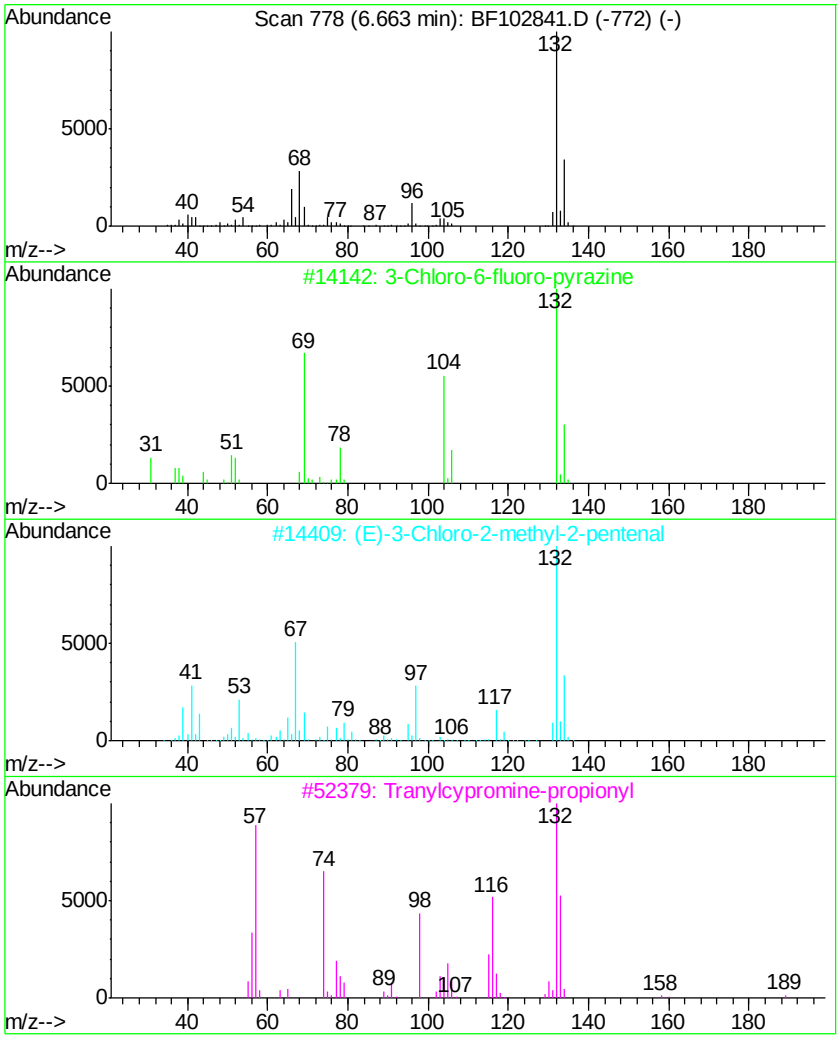
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

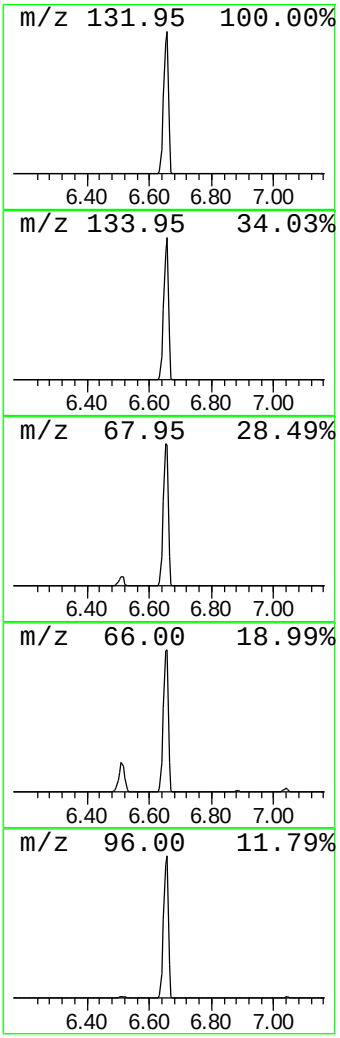
**********

Peak Number 3 unknown6.66 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.66 | 88.80 ng | 4333060 | 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 | 35 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 17 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 4 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 5 | 1,3,5-Trifluorobenzene | 132 | C6H3F3 | 000372-38-3 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020718\
Data File : BF102841.D
Acq On : 8 Feb 2018 3:31
Operator : SJ/JU
Sample : J1458-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-02

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

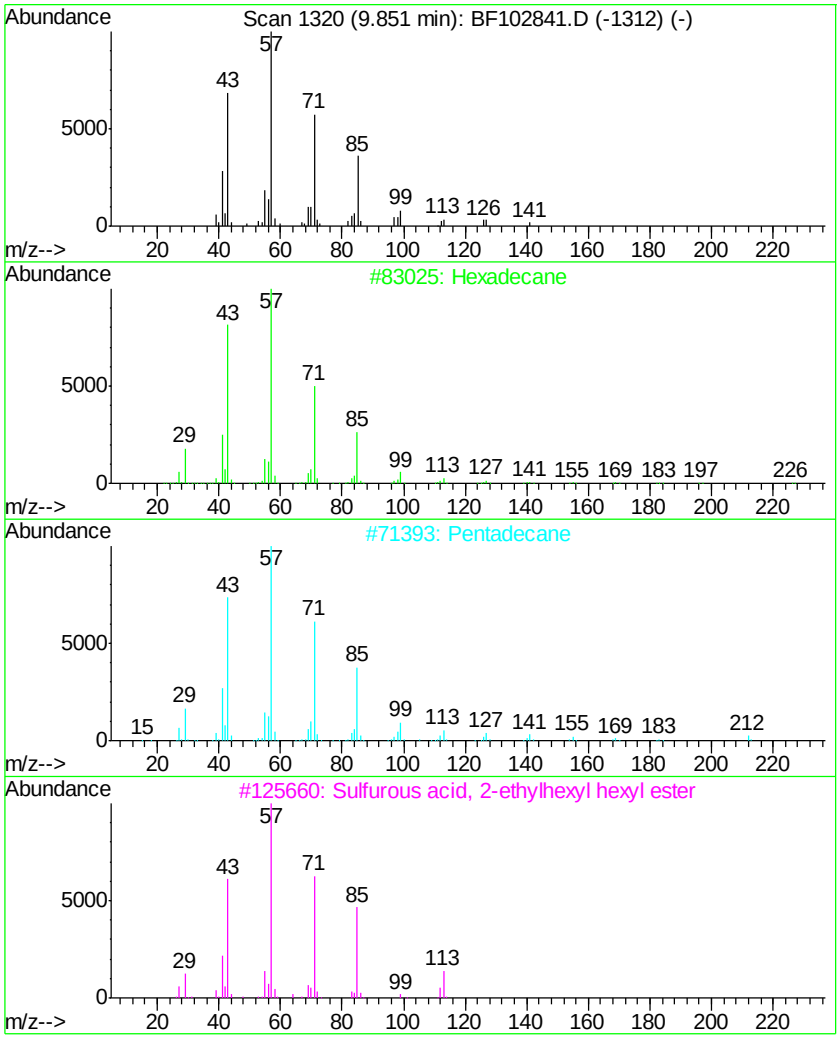
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

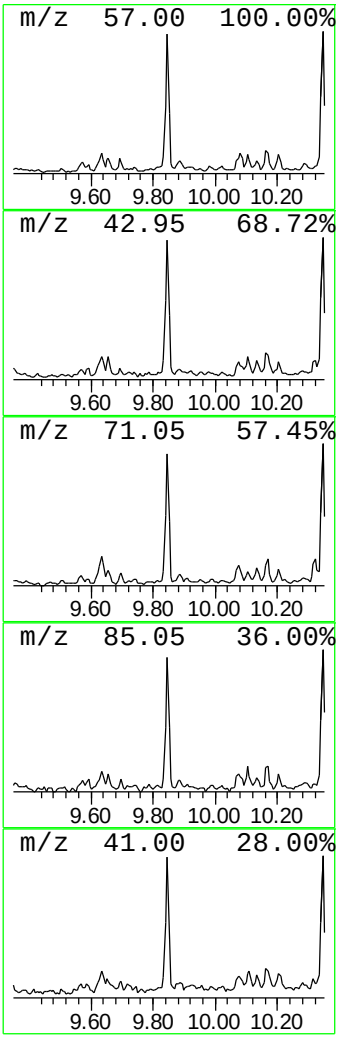
**********

Peak Number 5 Hexadecane Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.85 | 2.93 ng | 167575 | Acenaphthene-d10 | 9.92 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecane | 226 | C16H34 | 000544-76-3 | 87 |
| 2 | Pentadecane | 212 | C15H32 | 000629-62-9 | 83 |
| 3 | Sulfurous acid, 2-ethylhexyl hex... | 278 | C14H30O3S | 1000309-20-2 | 80 |
| 4 | Tridecane | 184 | C13H28 | 000629-50-5 | 72 |
| 5 | Decane, 2,9-dimethyl- | 170 | C12H26 | 001002-17-1 | 64 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020718\
Data File : BF102841.D
Acq On : 8 Feb 2018 3:31
Operator : SJ/JU
Sample : J1458-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-02

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

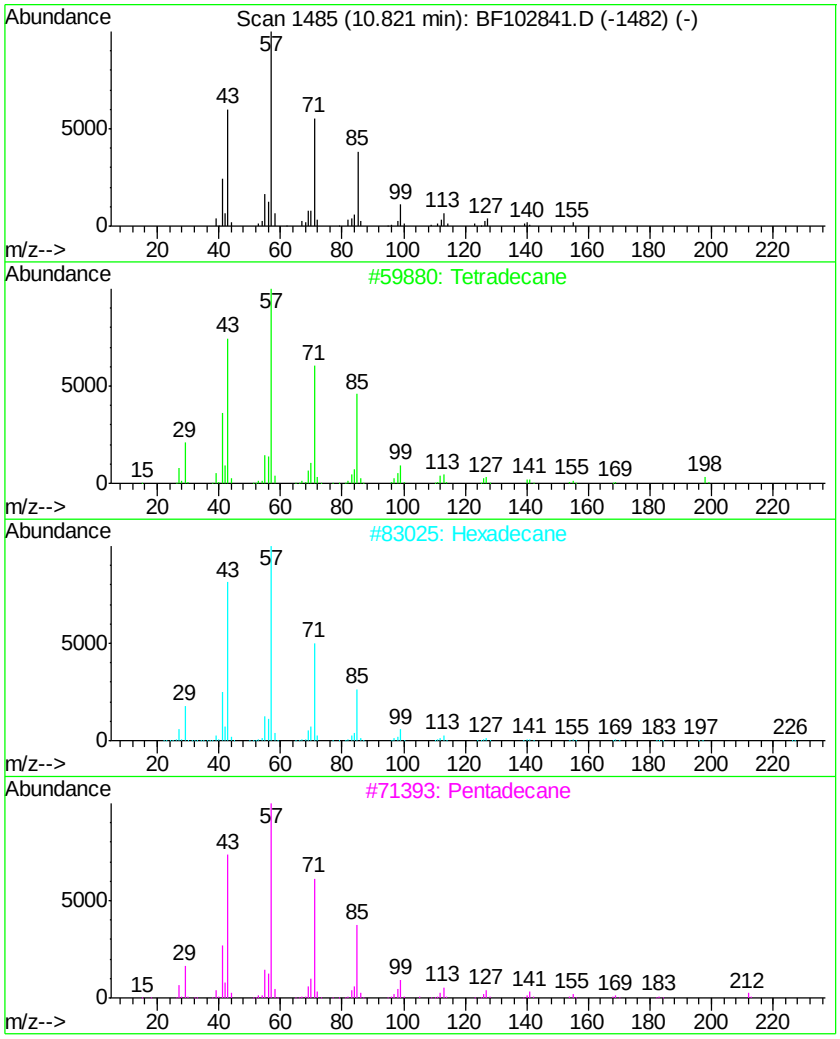
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

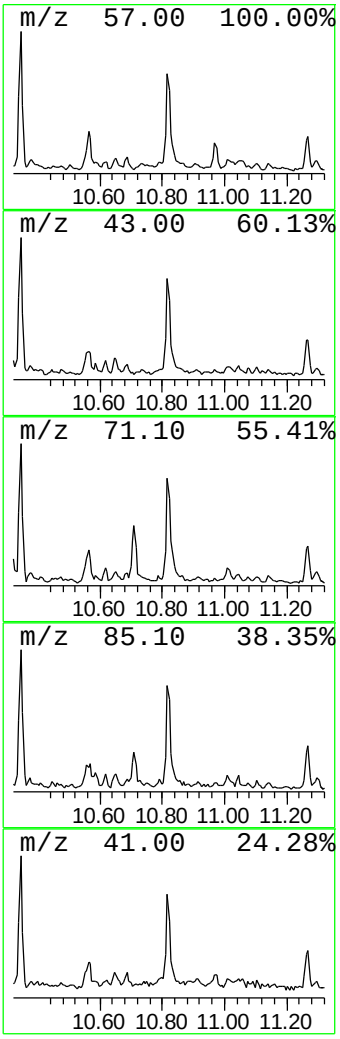
**********

Peak Number 7 Tetradecane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.82 | 3.56 ng | 165145 | Phenanthrene-d10 | 11.41 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetradecane | 198 | C14H30 | 000629-59-4 | 90 |
| 2 | Hexadecane | 226 | C16H34 | 000544-76-3 | 90 |
| 3 | Pentadecane | 212 | C15H32 | 000629-62-9 | 86 |
| 4 | Sulfurous acid, 2-ethylhexyl hex... | 278 | C14H30O3S | 1000309-20-2 | 86 |
| 5 | Nonadecane, 9-methyl- | 282 | C20H42 | 013287-24-6 | 86 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020718\
Data File : BF102841.D
Acq On : 8 Feb 2018 3:31
Operator : SJ/JU
Sample : J1458-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-02

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

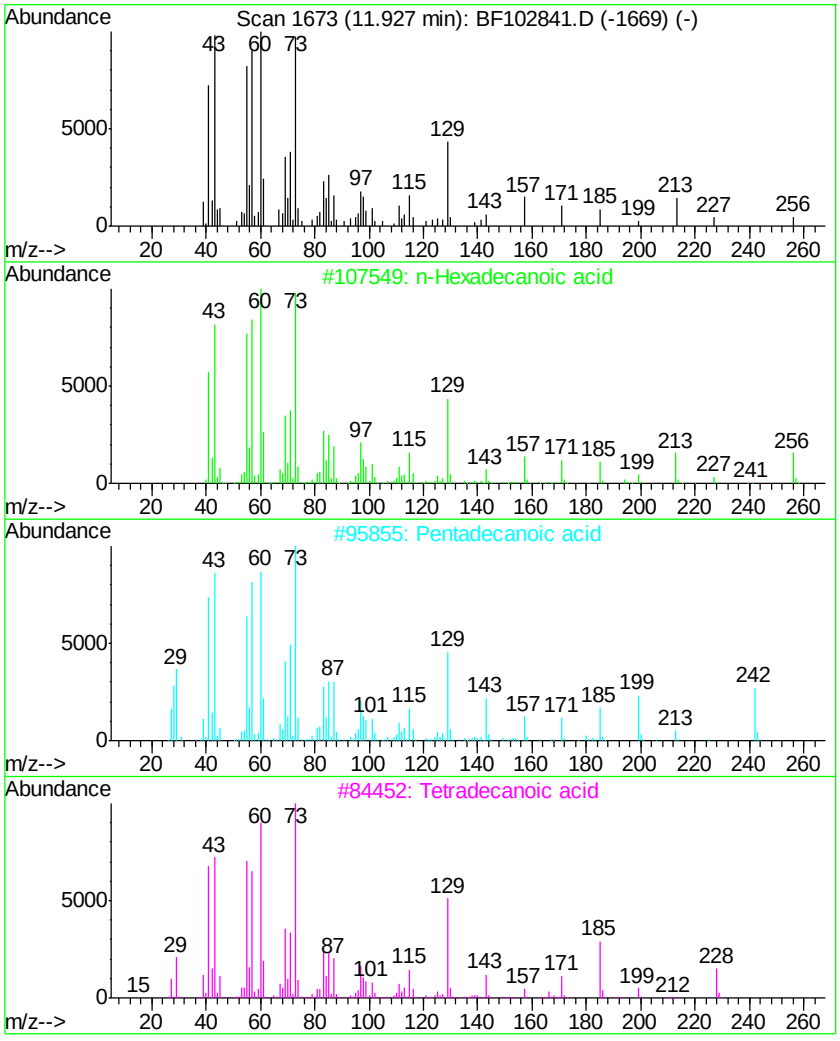
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

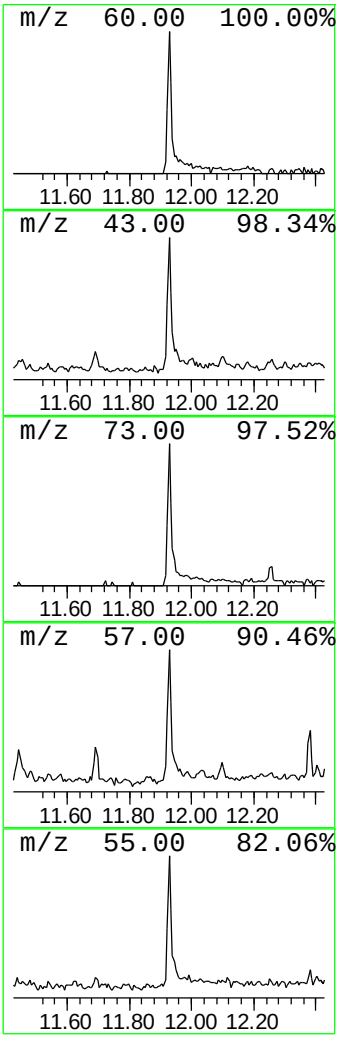
**********

Peak Number 8 n-Hexadecanoic acid Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.93 | 3.63 ng | 168217 | Phenanthrene-d10 | 11.41 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 91 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 83 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 72 |
| 4 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 64 |
| 5 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 59 |



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Data File : BF102841.D
Acq On : 8 Feb 2018 3:31
Operator : SJ/JU
Sample : J1458-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-02

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

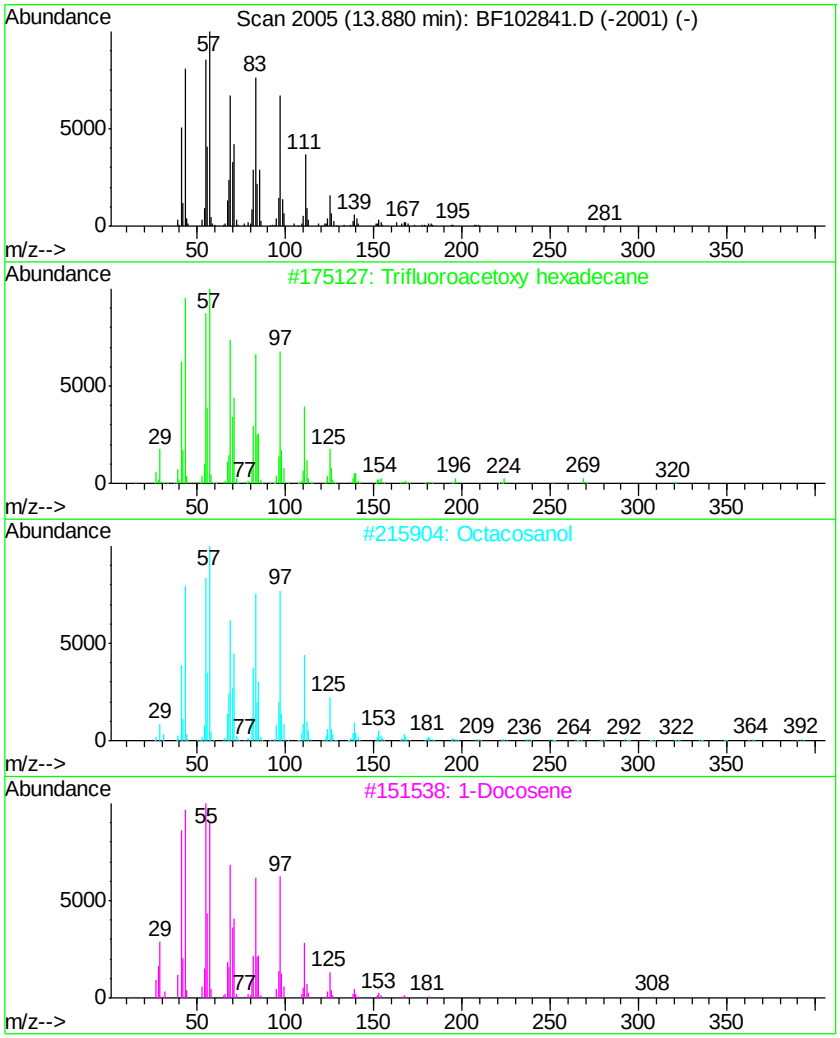
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

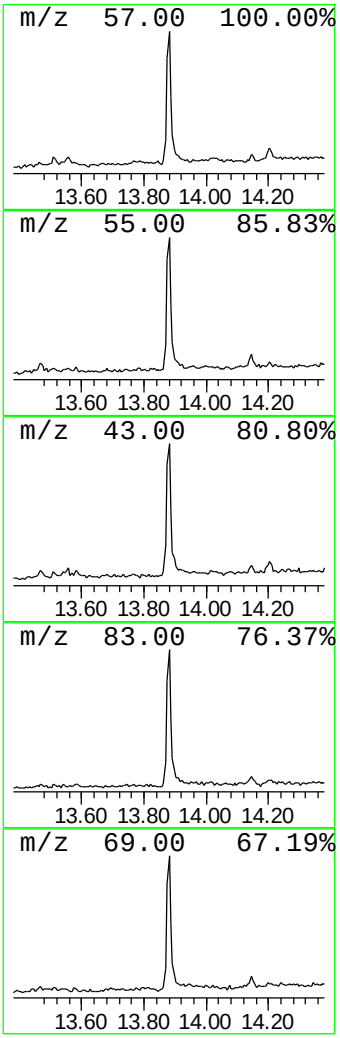
**********

Peak Number 9 Trifluoroacetoxy hexadecane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.88 | 10.06 ng | 444228 | Chrysene-d12 | 14.05 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 95 |
| 2 | Octacosanol | 410 | C28H58O | 000557-61-9 | 94 |
| 3 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 94 |
| 4 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 94 |
| 5 | Heptadecyl trifluoroacetate | 352 | C19H35F3O2 | 1000351-87-0 | 93 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020718\
Data File : BF102841.D
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Operator : SJ/JU
Sample : J1458-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** SB-02

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... | 2.18 | 11.5 | ng | 562890 | 1 | 6.89 | 975952 | 20.0 |
| 2-Pentanone, 4-hy... | 5.12 | 3.0 | ng | 145091 | 1 | 6.89 | 975952 | 20.0 |
| unknown6.66 | 6.66 | 88.8 | ng | 4333060 | 1 | 6.89 | 975952 | 20.0 |
| Hexadecane | 9.85 | 2.9 | ng | 167575 | 3 | 9.92 | 1142440 | 20.0 |
| Tetradecane | 10.82 | 3.6 | ng | 165145 | 4 | 11.41 | 927799 | 20.0 |
| n-Hexadecanoic acid | 11.93 | 3.6 | ng | 168217 | 4 | 11.41 | 927799 | 20.0 |
| Trifluoroacetoxy ... | 13.88 | 10.1 | ng | 444228 | 5 | 14.05 | 882794 | 20.0 |