LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
Data File : BF099556.D
Acq On : 16 Oct 2017 20:54
Operator : SJ/JU
Sample : I5782-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S2(10-12)

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-BF092317.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 | 2.257 | 26 | 29 | 45 | rVV | 117584 | 166454 | 5.45% | 0.660% |
| 2 | 2.404 | 47 | 54 | 62 | rVB | 214381 | 296554 | 9.71% | 1.177% |
| 3 | 4.457 | 400 | 403 | 420 | rVB | 46086 | 71019 | 2.33% | 0.282% |
| 4 | 4.610 | 425 | 429 | 435 | rBV | 31918 | 36788 | 1.20% | 0.146% |
| 5 | 4.857 | 467 | 471 | 477 | rVB | 111818 | 111644 | 3.66% | 0.443% |
| 6 | 5.075 | 504 | 508 | 523 | rBV | 464139 | 661267 | 21.66% | 2.623% |
| 7 | 5.475 | 571 | 576 | 579 | rBV | 2589632 | 2593223 | 84.94% | 10.288% |
| 8 | 6.487 | 743 | 748 | 766 | rBV | 2322938 | 2825106 | 92.53% | 11.208% |
| 9 | 6.616 | 766 | 770 | 774 | rBV | 2673348 | 2738300 | 89.69% | 10.864% |
| 10 | 6.845 | 805 | 809 | 815 | rBV | 664069 | 580648 | 19.02% | 2.304% |
| 11 | 6.998 | 831 | 835 | 839 | rBV | 2280759 | 2162648 | 70.83% | 8.580% |
| 12 | 7.410 | 900 | 905 | 908 | rBV | 1616147 | 1721483 | 56.38% | 6.830% |
| 13 | 8.122 | 1022 | 1026 | 1030 | rBV | 849652 | 804191 | 26.34% | 3.190% |
| 14 | 8.681 | 1118 | 1121 | 1129 | rBB | 42895 | 34886 | 1.14% | 0.138% |
| 15 | 9.198 | 1204 | 1209 | 1213 | rBV | 2967150 | 3053177 | 100.00% | 12.113% |
| 16 | 9.592 | 1272 | 1276 | 1281 | rBV | 734176 | 599378 | 19.63% | 2.378% |
| 17 | 9.880 | 1321 | 1325 | 1329 | rBV2 | 1067343 | 869488 | 28.48% | 3.449% |
| 18 | 10.592 | 1443 | 1446 | 1450 | rBV | 108993 | 85069 | 2.79% | 0.337% |
| 19 | 10.675 | 1456 | 1460 | 1463 | rBV | 1658430 | 1536342 | 50.32% | 6.095% |
| 20 | 11.369 | 1574 | 1578 | 1582 | rBV | 941783 | 786702 | 25.77% | 3.121% |
| 21 | 12.957 | 1843 | 1848 | 1851 | rBV | 2294030 | 2254470 | 73.84% | 8.944% |
| 22 | 13.833 | 1993 | 1997 | 2008 | rBV | 82892 | 115279 | 3.78% | 0.457% |
| 23 | 14.015 | 2024 | 2028 | 2035 | rVB | 564290 | 544591 | 17.84% | 2.161% |
| 24 | 15.486 | 2272 | 2278 | 2286 | rVB | 455911 | 557615 | 18.26% | 2.212% |

Sum of corrected areas: 25206322

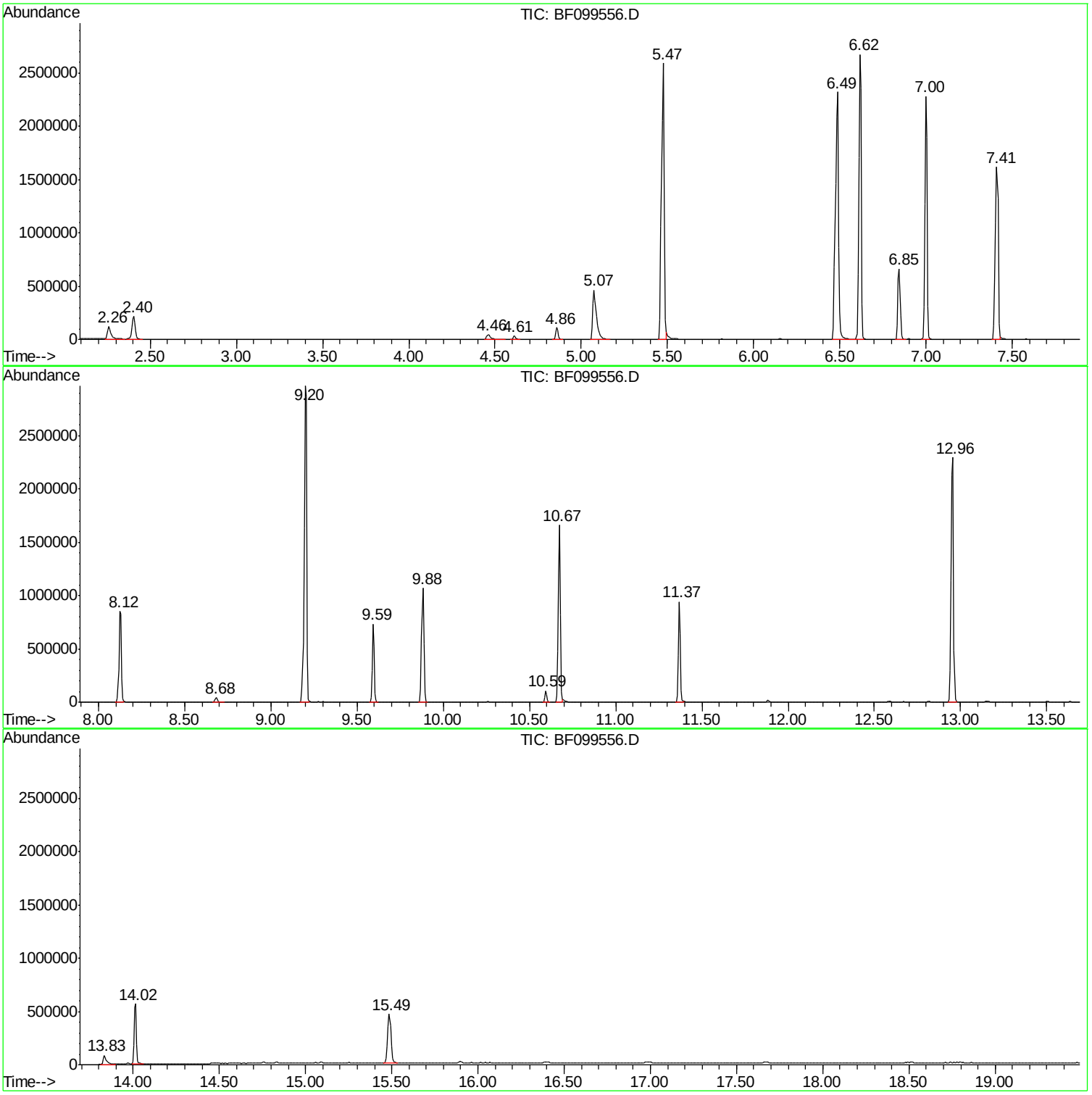
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
Data File : BF099556.D
Acq On : 16 Oct 2017 20:54
Operator : SJ/JU
Sample : I5782-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S2(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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\BF101617\
Data File : BF099556.D
Acq On : 16 Oct 2017 20:54
Operator : SJ/JU
Sample : I5782-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S2(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

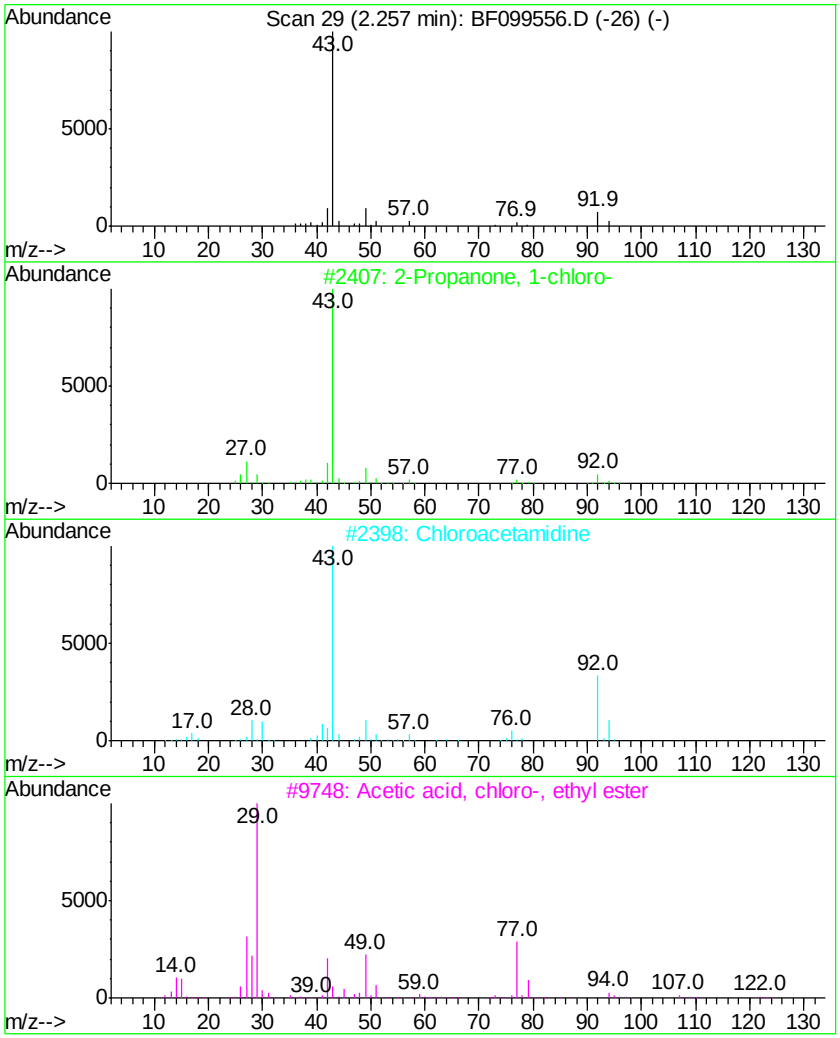
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

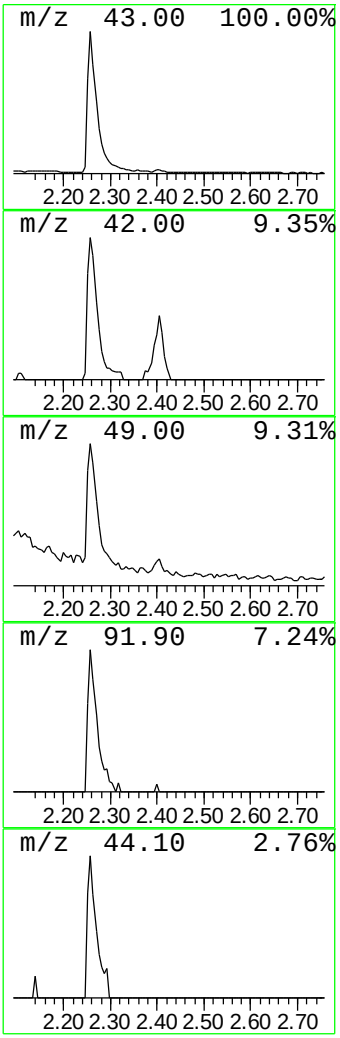
**********

Peak Number 1 2-Propanone, 1-chloro- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.26 | 5.73 ng | 166454 | 1,4-Dichlorobenzene-d4 | 6.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Propanone, 1-chloro- | 92 | C3H5ClO | 000078-95-5 | 91 |
| 2 | Chloroacetamidine | 92 | C2H5ClN2 | 020846-52-0 | 72 |
| 3 | Acetic acid, chloro-, ethyl ester | 122 | C4H7ClO2 | 000105-39-5 | 4 |
| 4 | Hydrogen azide | 43 | HN3 | 007782-79-8 | 4 |
| 5 | Acetyl chloride | 78 | C2H3ClO | 000075-36-5 | 4 |



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
Data File : BF099556.D
Acq On : 16 Oct 2017 20:54
Operator : SJ/JU
Sample : I5782-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S2(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

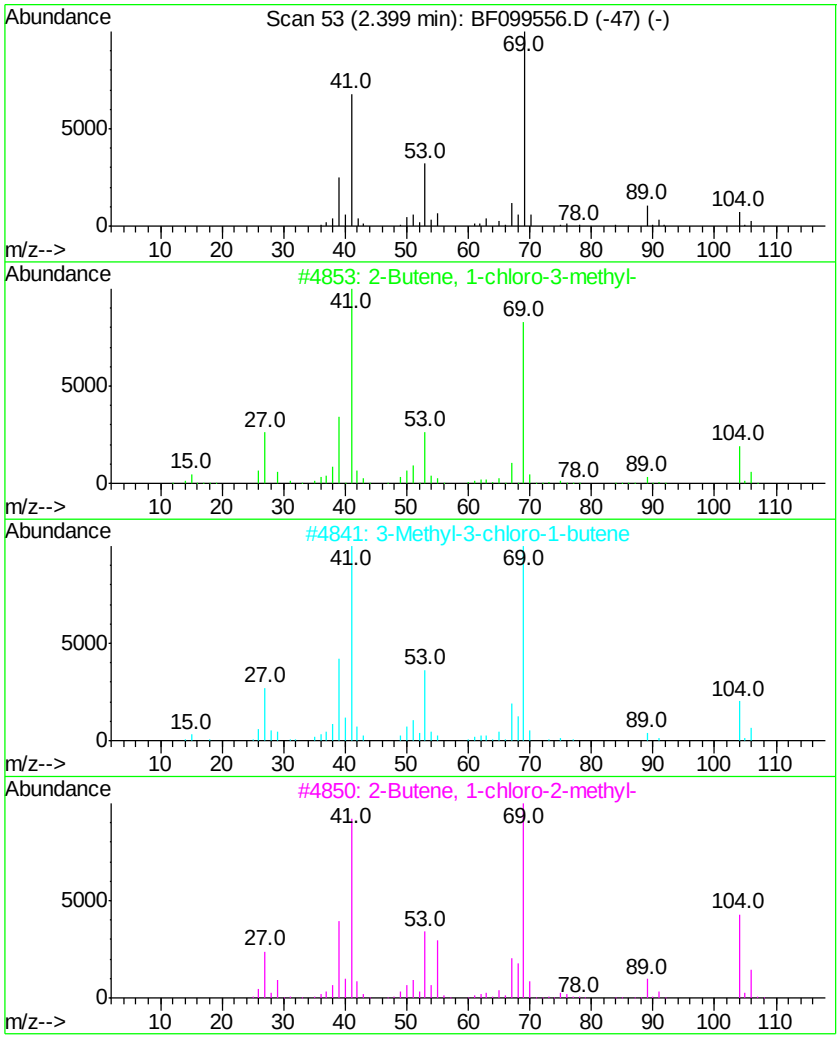
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

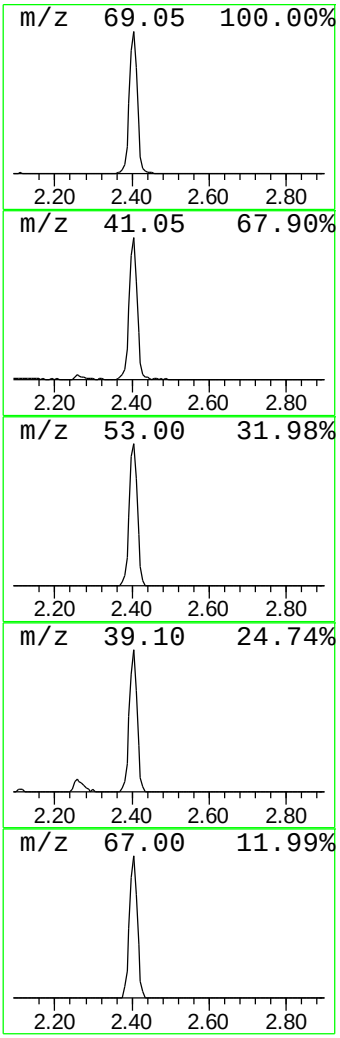
**********

Peak Number 2 2-Butene, 1-chloro-3-methyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.40 | 10.21 ng | 296554 | 1,4-Dichlorobenzene-d4 | 6.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Butene, 1-chloro-3-methyl- | 104 | C5H9Cl | 000503-60-6 | 72 |
| 2 | 3-Methyl-3-chloro-1-butene | 104 | C5H9Cl | 002190-48-9 | 50 |
| 3 | 2-Butene, 1-chloro-2-methyl- | 104 | C5H9Cl | 013417-43-1 | 50 |
| 4 | Trifluoroacetyl-lavandulol | 250 | C12H17F3O2 | 028673-24-7 | 42 |
| 5 | Cyclopentane, bromo- | 148 | C5H9Br | 000137-43-9 | 40 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
Data File : BF099556.D
Acq On : 16 Oct 2017 20:54
Operator : SJ/JU
Sample : I5782-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S2(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

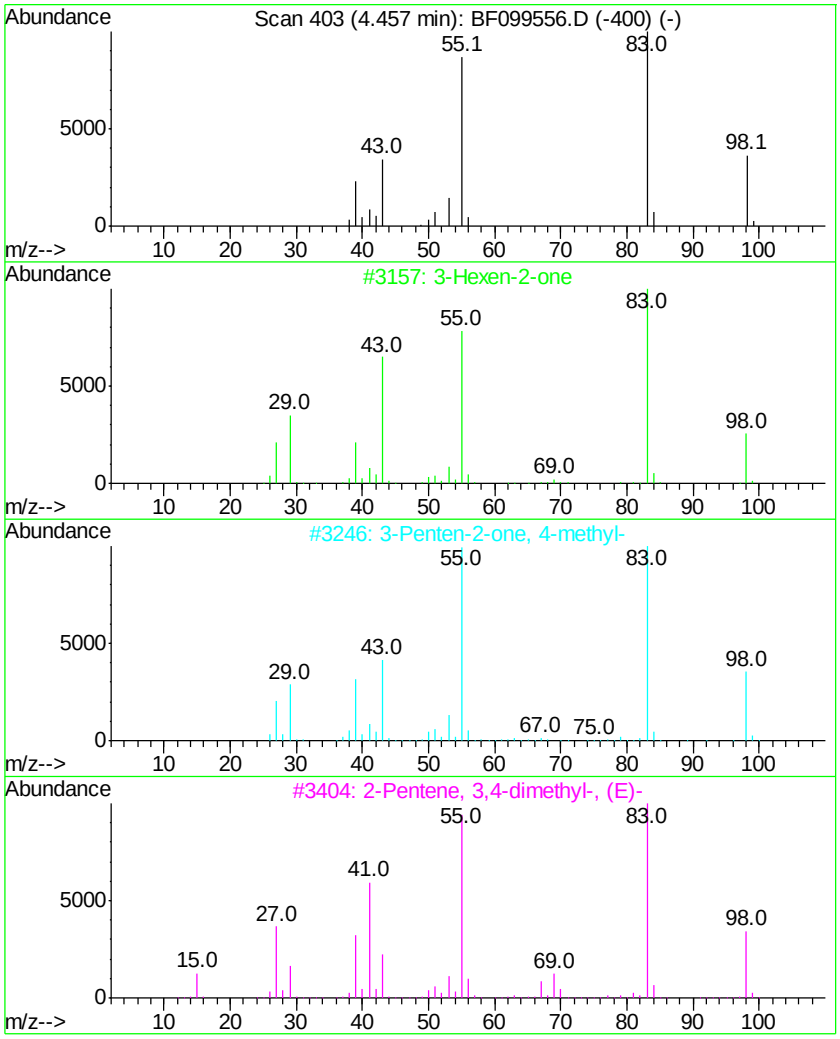
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

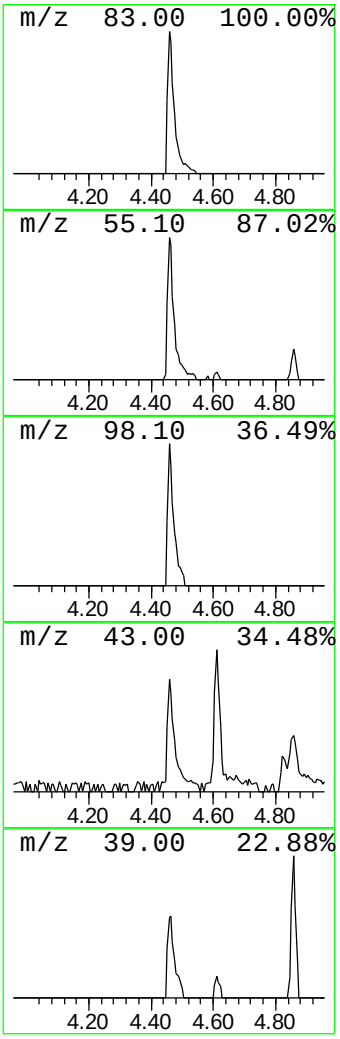
**********

Peak Number 3 3-Hexen-2-one Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.46 | 2.45 ng | 71019 | 1,4-Dichlorobenzene-d4 | 6.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Hexen-2-one | 98 | C6H10O | 000763-93-9 | 91 |
| 2 | 3-Penten-2-one, 4-methyl- | 98 | C6H10O | 000141-79-7 | 91 |
| 3 | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14 | 004914-92-5 | 90 |
| 4 | 2-Pentene, 4,4-dimethyl-, (Z)- | 98 | C7H14 | 000762-63-0 | 86 |
| 5 | 2-Pentene, 2,4-dimethyl- | 98 | C7H14 | 000625-65-0 | 86 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
Data File : BF099556.D
Acq On : 16 Oct 2017 20:54
Operator : SJ/JU
Sample : I5782-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S2(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

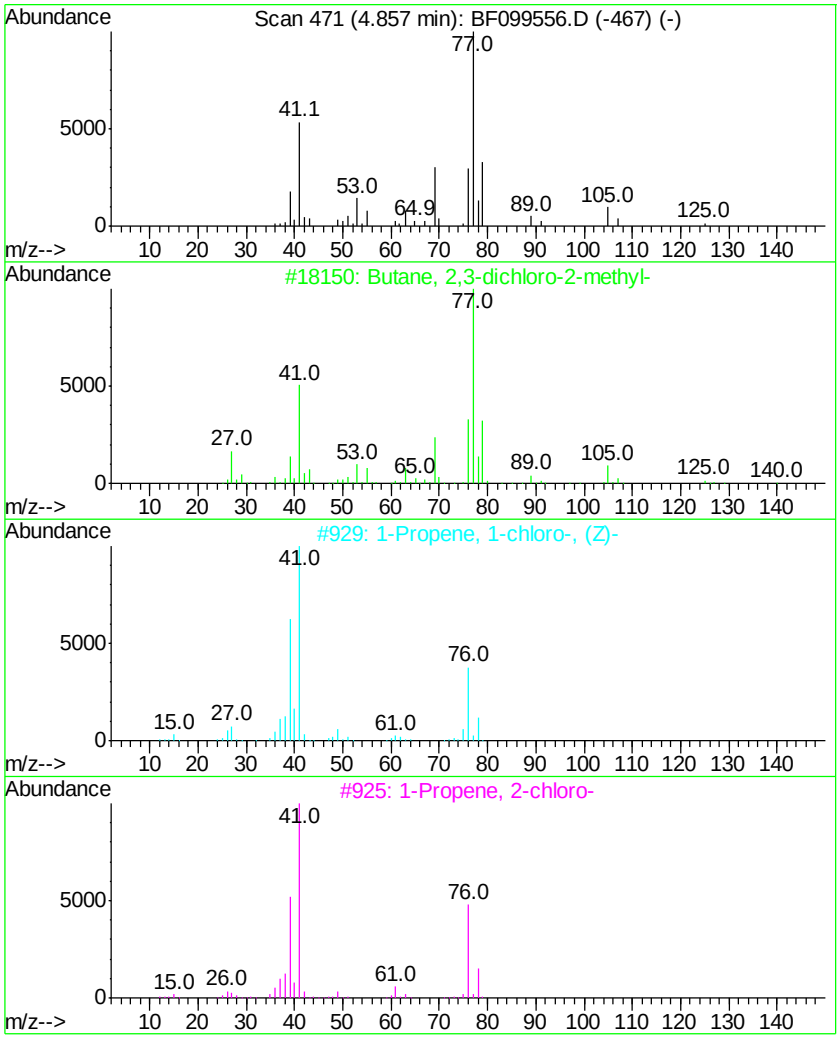
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

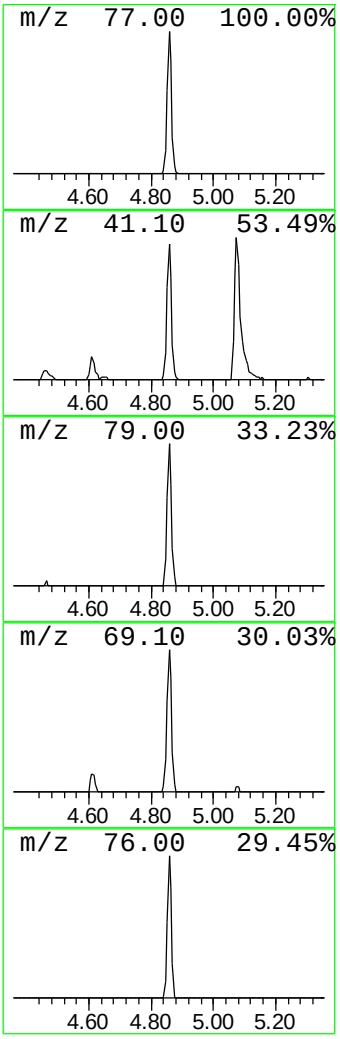
**********

Peak Number 4 Butane, 2,3-dichloro-2-methyl- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.86 | 3.85 ng | 111644 | 1,4-Dichlorobenzene-d4 | 6.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2,3-dichloro-2-methyl- | 140 | C5H10Cl2 | 000507-45-9 | 90 |
| 2 | 1-Propene, 1-chloro-, (Z)- | 76 | C3H5Cl | 016136-84-8 | 10 |
| 3 | 1-Propene, 2-chloro- | 76 | C3H5Cl | 000557-98-2 | 9 |
| 4 | Allyl chloride | 76 | C3H5Cl | 000107-05-1 | 9 |
| 5 | Propane, 2-bromo-1-chloro- | 156 | C3H6BrCl | 003017-95-6 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
Data File : BF099556.D
Acq On : 16 Oct 2017 20:54
Operator : SJ/JU
Sample : I5782-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S2(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

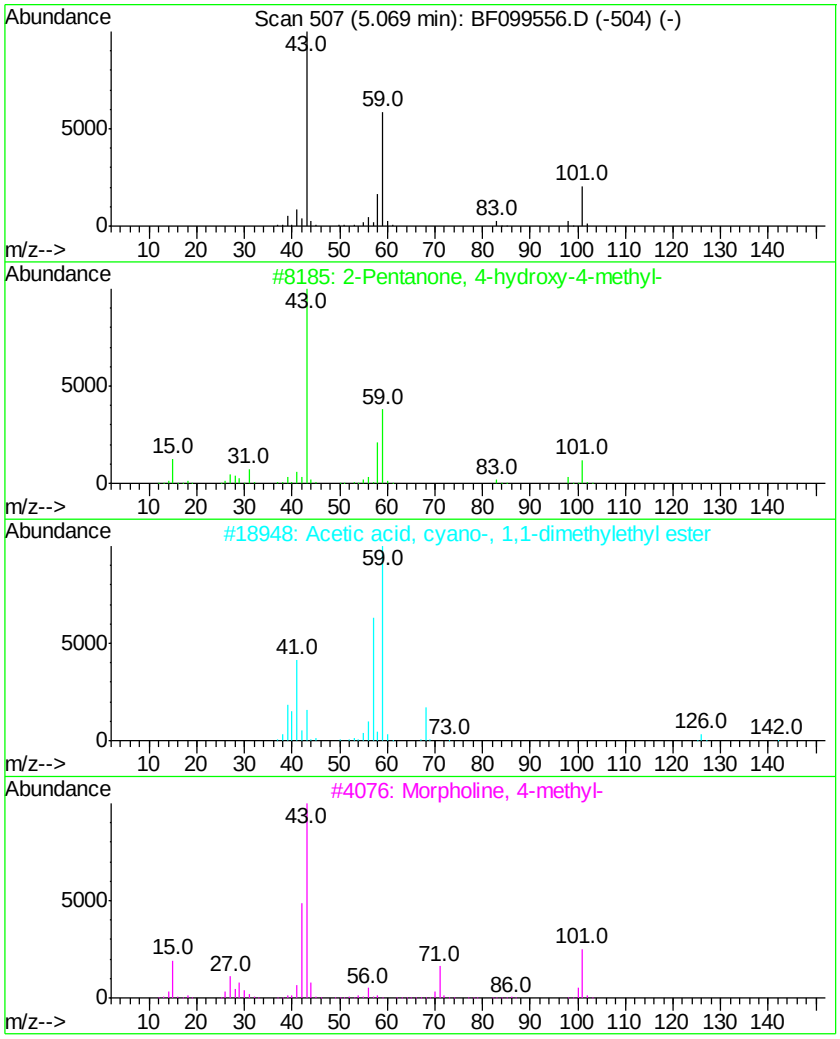
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

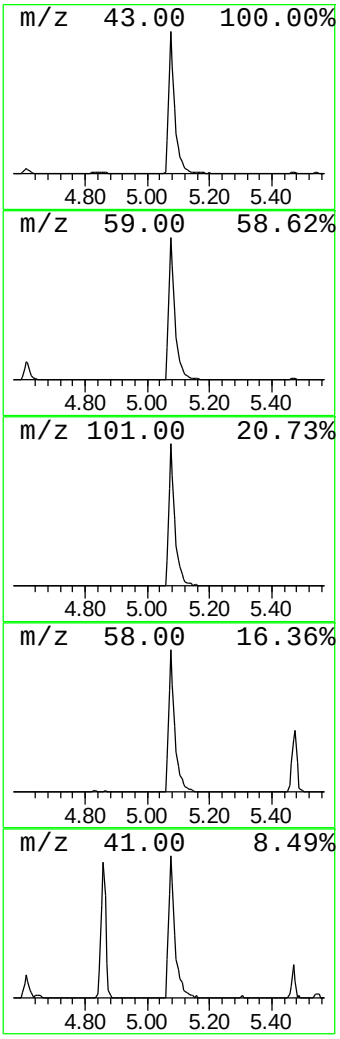
**********

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.07 | 22.78 ng | 661267 | 1,4-Dichlorobenzene-d4 | 6.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 72 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17 |
| 3 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 9 |
| 5 | Acetone | 58 | C3H6O | 000067-64-1 | 9 |



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Data File : BF099556.D
Acq On : 16 Oct 2017 20:54
Operator : SJ/JU
Sample : I5782-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S2(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

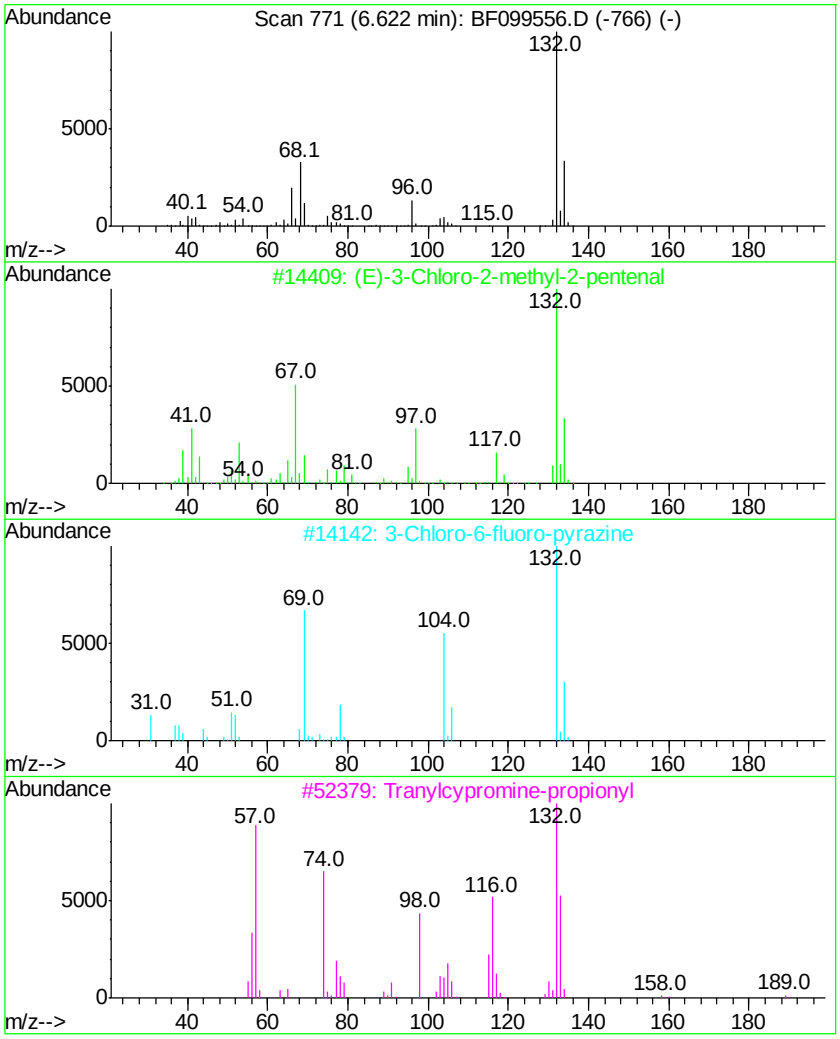
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

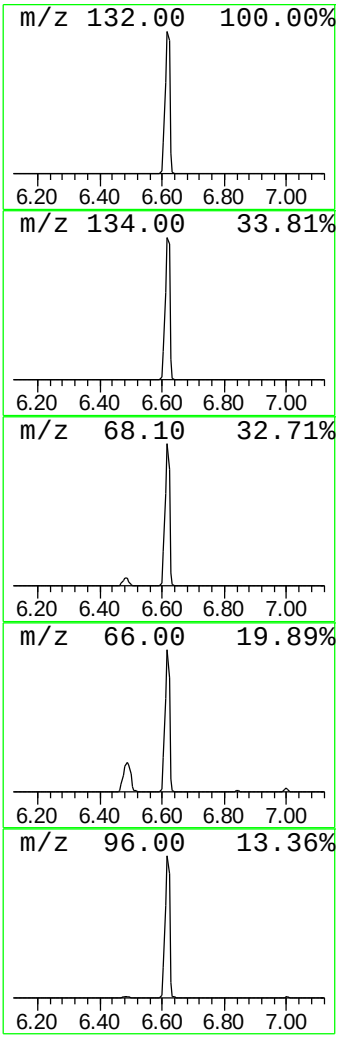
**********

Peak Number 6 unknown6.62 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.62 | 94.32 ng | 2738300 | 1,4-Dichlorobenzene-d4 | 6.85 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 35 |
| 2 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 25 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 12 |
| 4 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 5 | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2 | 022291-85-6 | 9 |



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Data File : BF099556.D
Acq On : 16 Oct 2017 20:54
Operator : SJ/JU
Sample : I5782-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S2(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

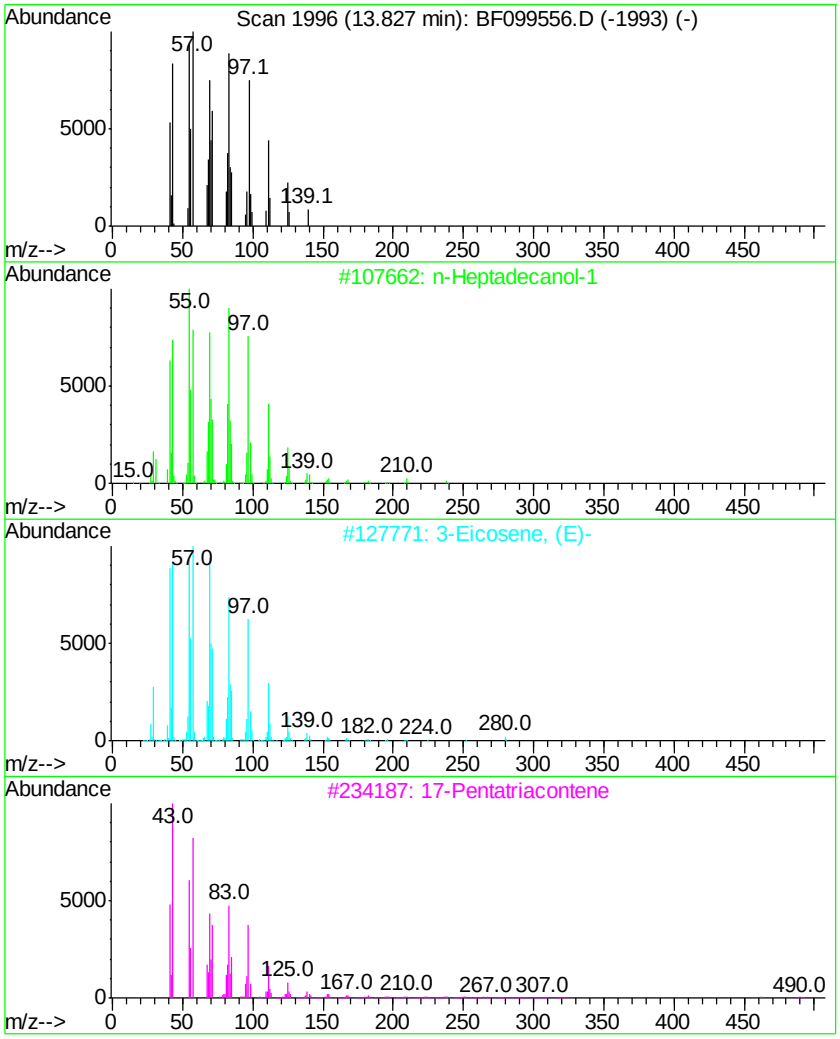
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

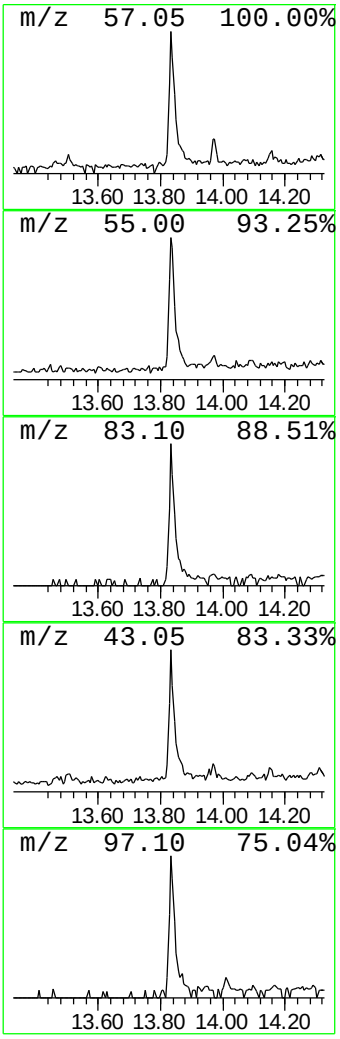
**********

Peak Number 8 n-Heptadecanol-1 Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.83 | 4.23 ng | 115279 | Chrysene-d12 | 14.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Heptadecanol-1 | 256 | C17H36O | 001454-85-9 | 87 |
| 2 | 3-Eicosene, (E)- | 280 | C20H40 | 074685-33-9 | 87 |
| 3 | 17-Pentatriacontene | 491 | C35H70 | 006971-40-0 | 86 |
| 4 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 81 |
| 5 | 1-Docosene | 308 | C22H44 | 001599-67-3 | 81 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101617\
Data File : BF099556.D
Acq On : 16 Oct 2017 20:54
Operator : SJ/JU
Sample : I5782-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S2(10-12)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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-Propanone, 1-ch... | 2.26 | 5.7 | ng | 166454 | 1 | 6.85 | 580648 | 20.0 |
| 2-Butene, 1-chlor... | 2.40 | 10.2 | ng | 296554 | 1 | 6.85 | 580648 | 20.0 |
| 3-Hexen-2-one | 4.46 | 2.5 | ng | 71019 | 1 | 6.85 | 580648 | 20.0 |
| Butane, 2,3-dichl... | 4.86 | 3.9 | ng | 111644 | 1 | 6.85 | 580648 | 20.0 |
| 2-Pentanone, 4-hy... | 5.07 | 22.8 | ng | 661267 | 1 | 6.85 | 580648 | 20.0 |
| unknown6.62 | 6.62 | 94.3 | ng | 2738300 | 1 | 6.85 | 580648 | 20.0 |
| n-Heptadecanol-1 | 13.83 | 4.2 | ng | 115279 | 5 | 14.02 | 544591 | 20.0 |