LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096616.D
Acq On : 10 Jul 2017 22:16
Operator : SJ/JU
Sample : I4078-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** VNJ-211

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-BF070117.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 | 4.875 | 469 | 474 | 487 | rVB | 426016 | 614370 | 20.12% | 2.432% |
| 2 | 5.298 | 541 | 546 | 549 | rBV | 2874732 | 2932092 | 96.02% | 11.605% |
| 3 | 6.328 | 715 | 721 | 725 | rBV | 2663373 | 3053645 | 100.00% | 12.086% |
| 4 | 6.451 | 738 | 742 | 746 | rBV | 2803995 | 2973591 | 97.38% | 11.769% |
| 5 | 6.681 | 778 | 781 | 785 | rBV | 899033 | 762665 | 24.98% | 3.019% |
| 6 | 6.839 | 801 | 808 | 811 | rBV | 2517003 | 2286441 | 74.88% | 9.049% |
| 7 | 7.245 | 871 | 877 | 880 | rBV | 1969024 | 1913973 | 62.68% | 7.575% |
| 8 | 7.963 | 995 | 999 | 1003 | rBV | 1275599 | 1067490 | 34.96% | 4.225% |
| 9 | 9.045 | 1177 | 1183 | 1186 | rBV | 2848910 | 2720363 | 89.09% | 10.767% |
| 10 | 9.433 | 1245 | 1249 | 1252 | rBV | 401499 | 302299 | 9.90% | 1.196% |
| 11 | 9.716 | 1291 | 1297 | 1305 | rBV | 1060357 | 990524 | 32.44% | 3.920% |
| 12 | 10.163 | 1370 | 1373 | 1376 | rVB | 53341 | 42944 | 1.41% | 0.170% |
| 13 | 10.498 | 1426 | 1430 | 1433 | rBV | 1465052 | 1307666 | 42.82% | 5.176% |
| 14 | 10.633 | 1450 | 1453 | 1461 | rBV | 61505 | 77862 | 2.55% | 0.308% |
| 15 | 11.080 | 1525 | 1529 | 1532 | rBV2 | 40306 | 36819 | 1.21% | 0.146% |
| 16 | 11.192 | 1544 | 1548 | 1551 | rBV | 812897 | 680173 | 22.27% | 2.692% |
| 17 | 11.733 | 1637 | 1640 | 1643 | rBV2 | 46241 | 41697 | 1.37% | 0.165% |
| 18 | 12.774 | 1813 | 1817 | 1821 | rBV | 1688727 | 1580788 | 51.77% | 6.257% |
| 19 | 12.957 | 1846 | 1848 | 1853 | rBV6 | 35561 | 45017 | 1.47% | 0.178% |
| 20 | 13.257 | 1897 | 1899 | 1902 | rVB | 40469 | 30756 | 1.01% | 0.122% |
| 21 | 13.680 | 1968 | 1971 | 1977 | rVB | 168353 | 165874 | 5.43% | 0.657% |
| 22 | 13.821 | 1991 | 1995 | 1998 | rBV | 626996 | 639509 | 20.94% | 2.531% |
| 23 | 15.221 | 2229 | 2233 | 2236 | rVB | 464702 | 491722 | 16.10% | 1.946% |
| 24 | 15.362 | 2255 | 2257 | 2264 | rVB3 | 139209 | 207527 | 6.80% | 0.821% |
| 25 | 15.710 | 2314 | 2316 | 2325 | rVB6 | 176977 | 300214 | 9.83% | 1.188% |

Sum of corrected areas: 25266021

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096616.D
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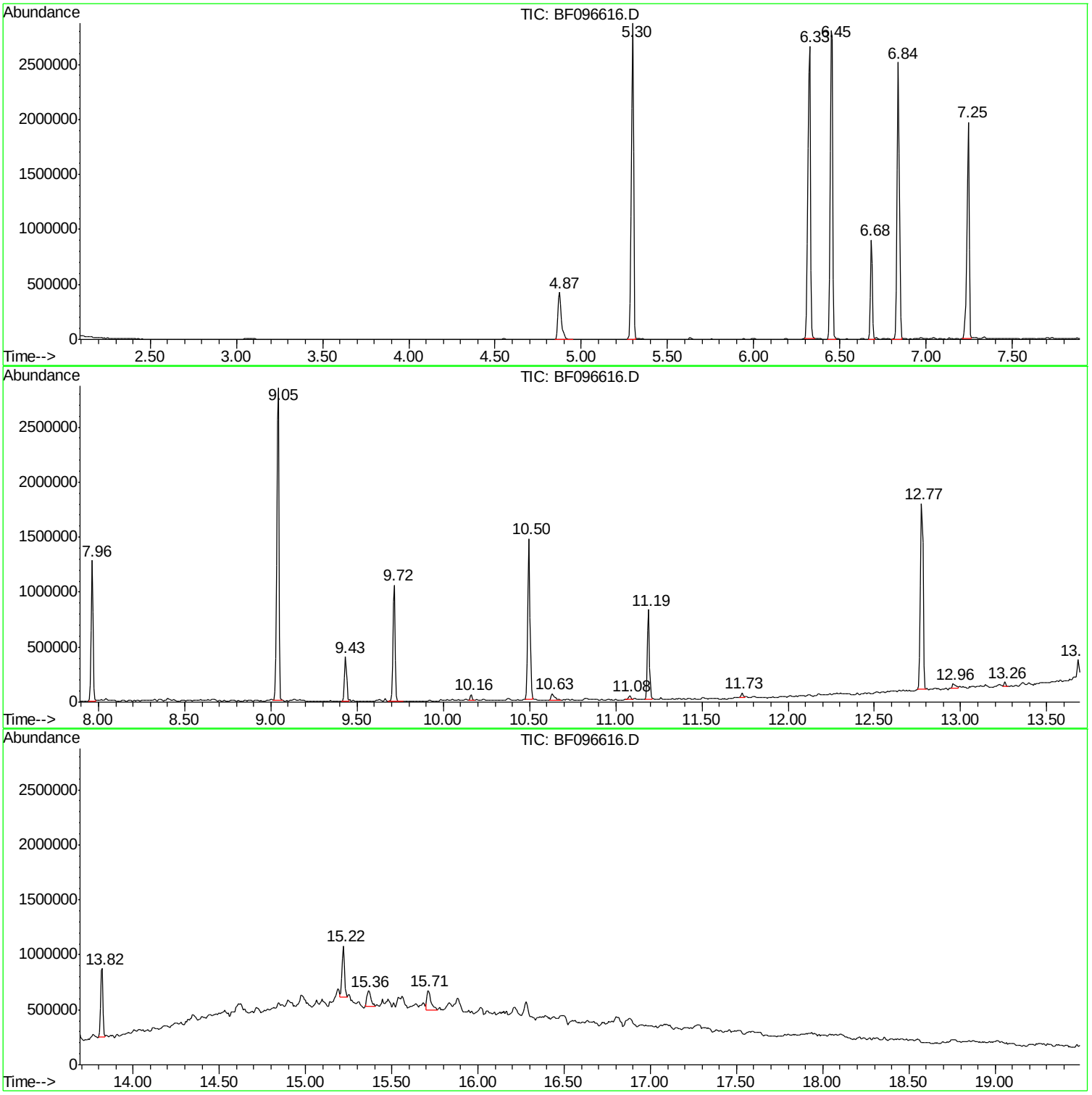
Operator : SJ/JU
Sample : I4078-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** VNJ-211

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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\BF071017\
Data File : BF096616.D
Acq On : 10 Jul 2017 22:16
Operator : SJ/JU
Sample : I4078-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** VNJ-211

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

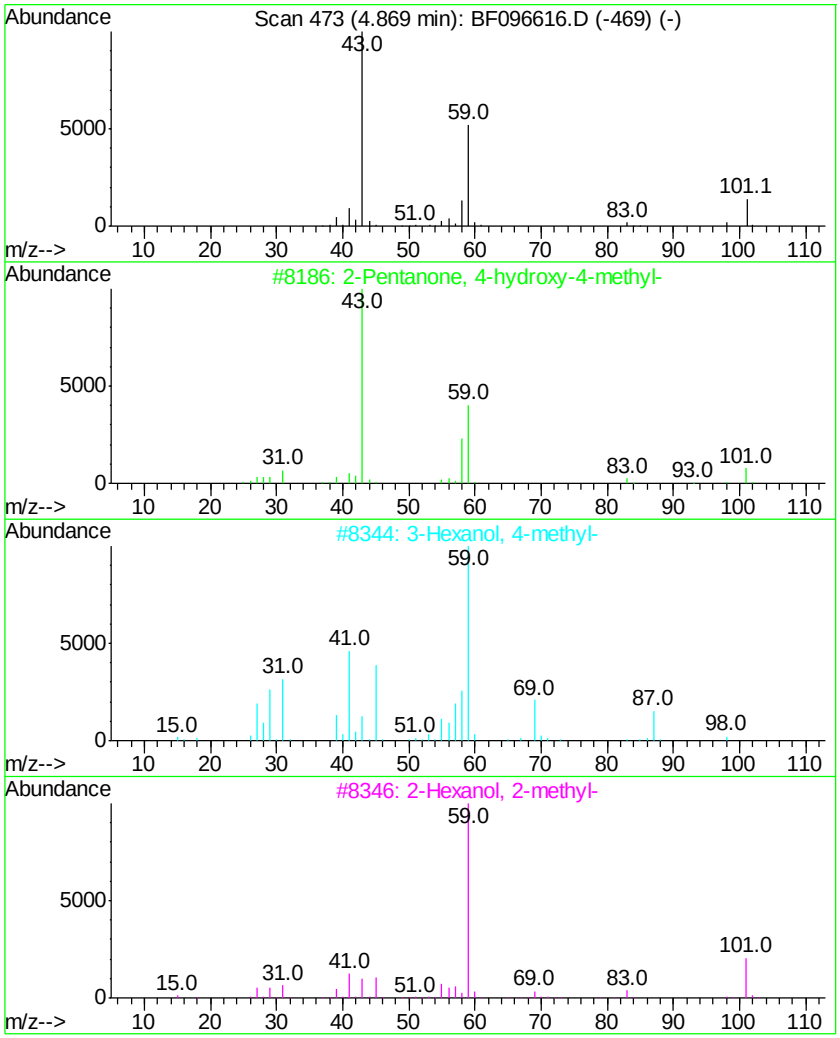
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

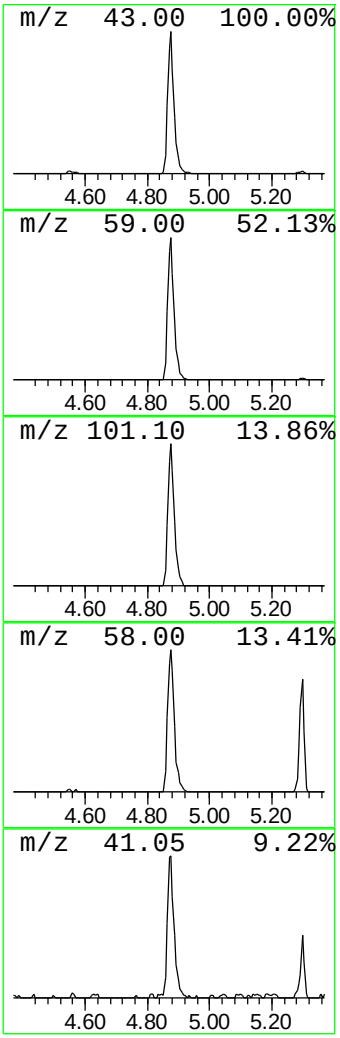
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.87 | 16.11 ng | 614370 | 1,4-Dichlorobenzene-d4 | 6.68 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 50 |
| 2 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 3 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 33 |
| 4 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |
| 5 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 10 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096616.D
Acq On : 10 Jul 2017 22:16
Operator : SJ/JU
Sample : I4078-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** VNJ-211

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

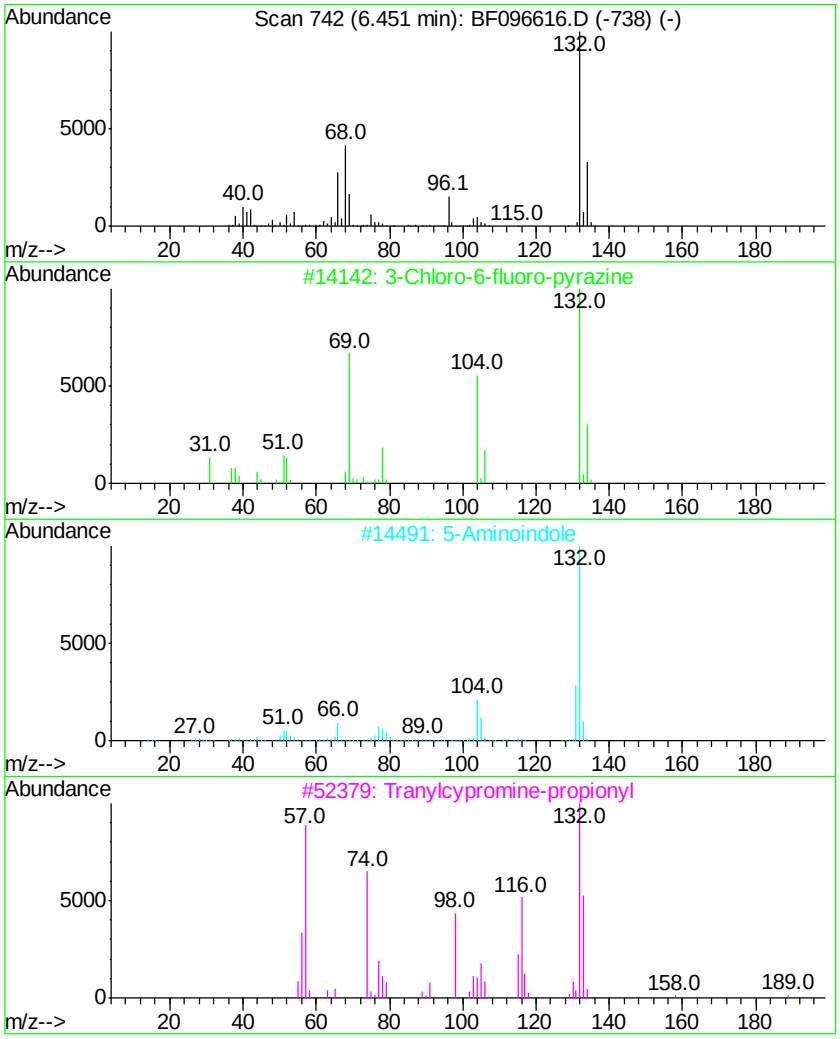
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

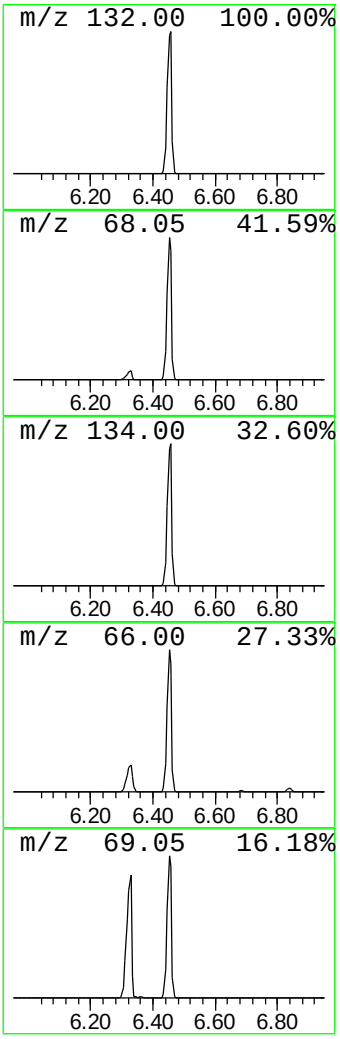
**********

Peak Number 2 unknown6.45 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.45 | 77.98 ng | 2973590 | 1,4-Dichlorobenzene-d4 | 6.68 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 5 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096616.D
Acq On : 10 Jul 2017 22:16
Operator : SJ/JU
Sample : I4078-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** VNJ-211

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

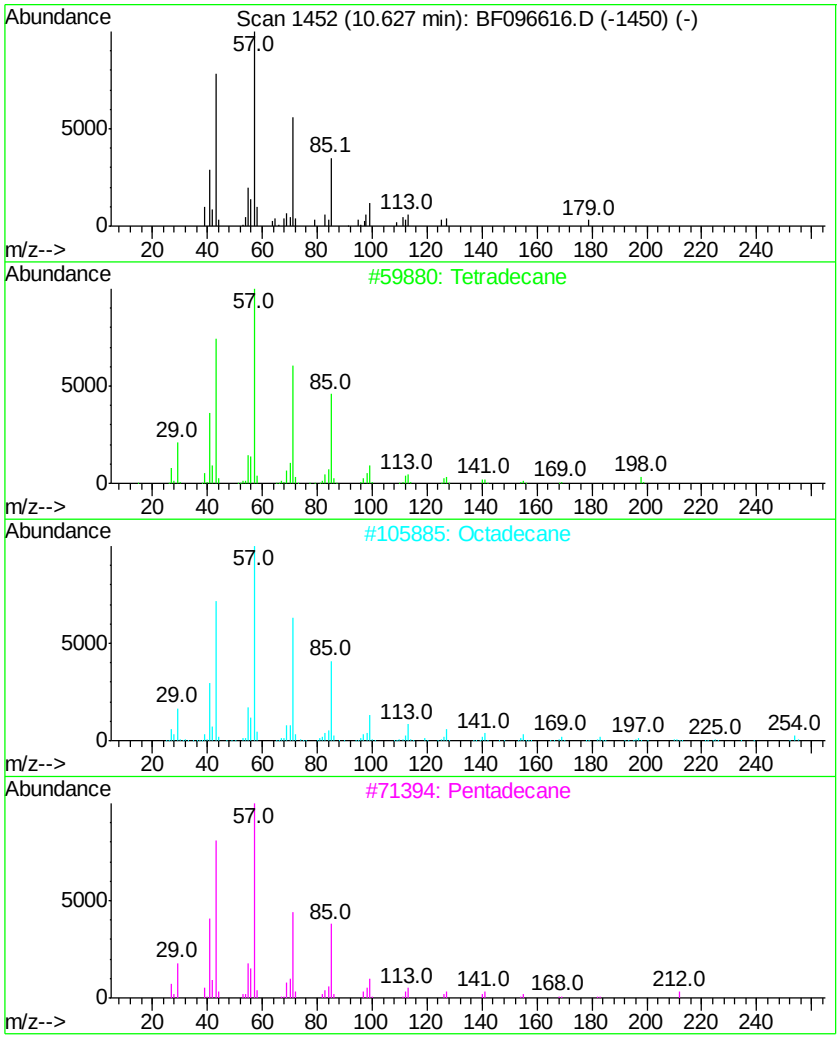
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

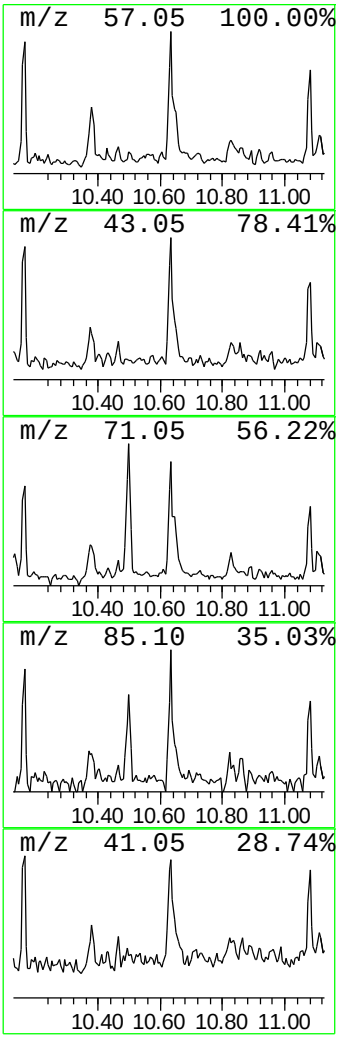
**********

Peak Number 4 Tetradecane Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.63 | 2.29 ng | 77862 | Phenanthrene-d10 | 11.19 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Tetradecane | 198 | C14H30 | 000629-59-4 | 90 |
| 2 | Octadecane | 254 | C18H38 | 000593-45-3 | 78 |
| 3 | Pentadecane | 212 | C15H32 | 000629-62-9 | 64 |
| 4 | Hexadecane | 226 | C16H34 | 000544-76-3 | 64 |
| 5 | Sulfurous acid, hexyl heptyl ester | 264 | C13H28O3S | 1000309-12-9 | 58 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096616.D
Acq On : 10 Jul 2017 22:16
Operator : SJ/JU
Sample : I4078-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** VNJ-211

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

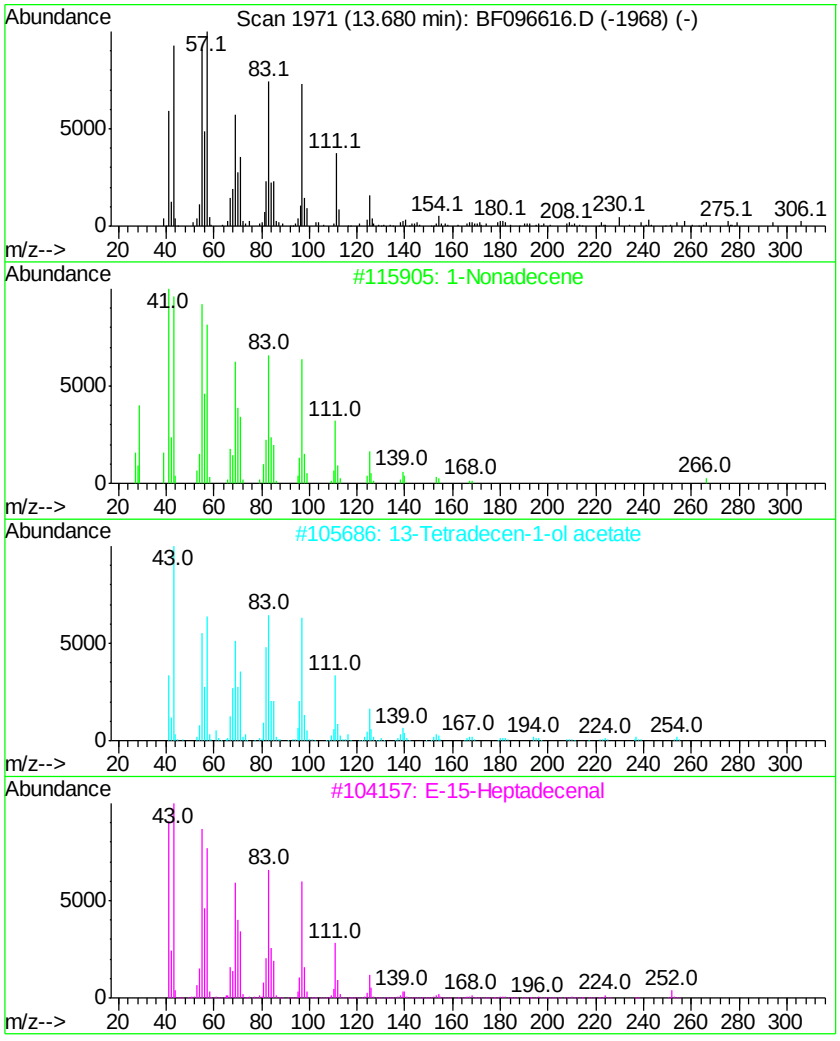
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

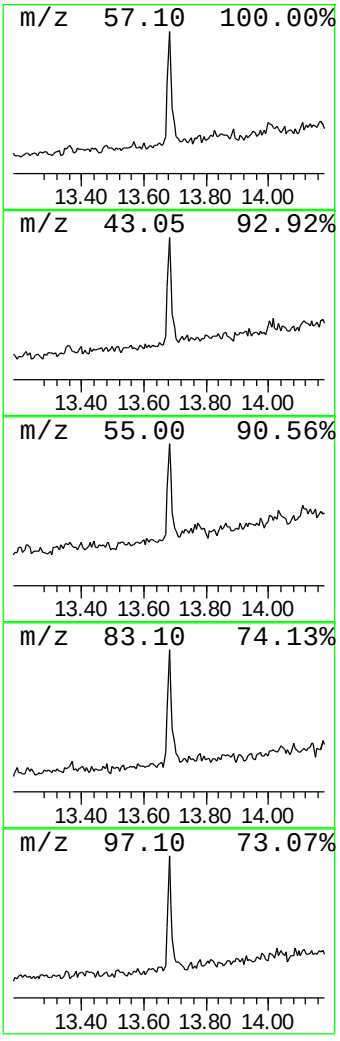
**********

Peak Number 5 1-Nonadecene Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.68 | 5.19 ng | 165874 | Chrysene-d12 | 13.82 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Nonadecene | 266 | C19H38 | 018435-45-5 | 94 |
| 2 | 13-Tetradecen-1-ol acetate | 254 | C16H30O2 | 056221-91-1 | 93 |
| 3 | E-15-Heptadecenal | 252 | C17H32O | 1000130-97-9 | 91 |
| 4 | 5-Eicosene, (E)- | 280 | C20H40 | 074685-30-6 | 90 |
| 5 | Trifluoroacetic acid,n-tridecyl ... | 296 | C15H27F3O2 | 053800-02-5 | 83 |



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Acq On : 10 Jul 2017 22:16
Operator : SJ/JU
Sample : I4078-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** VNJ-211

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

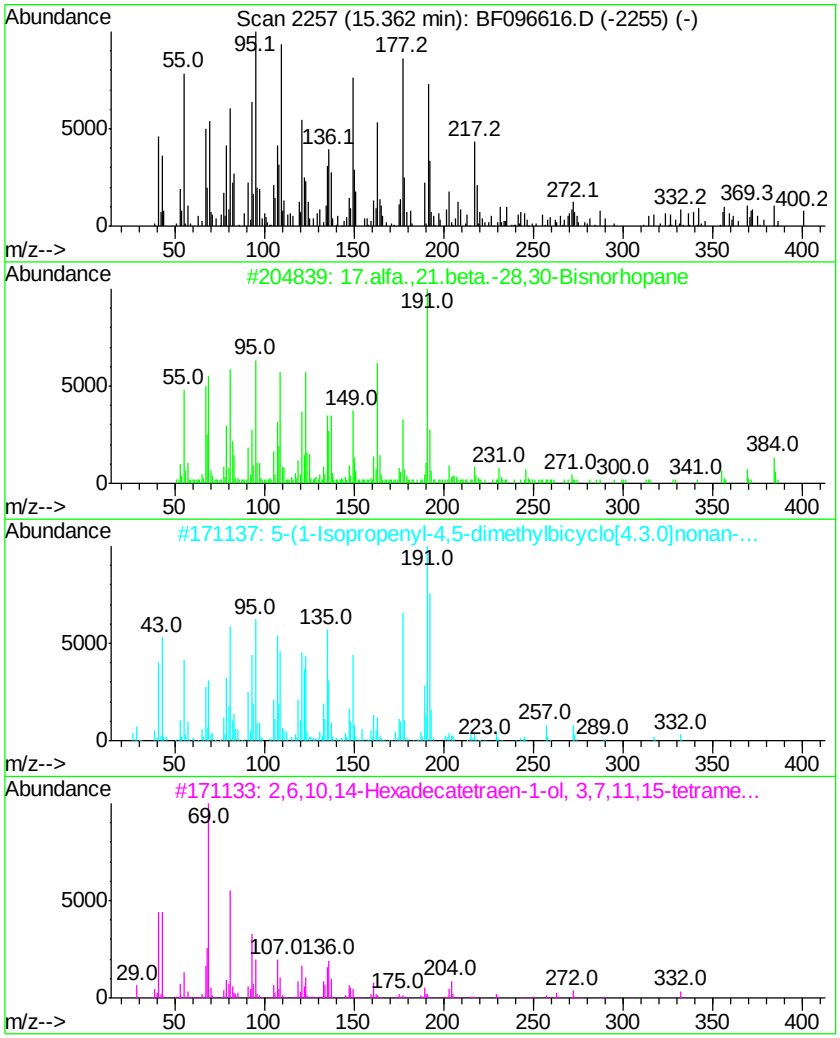
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

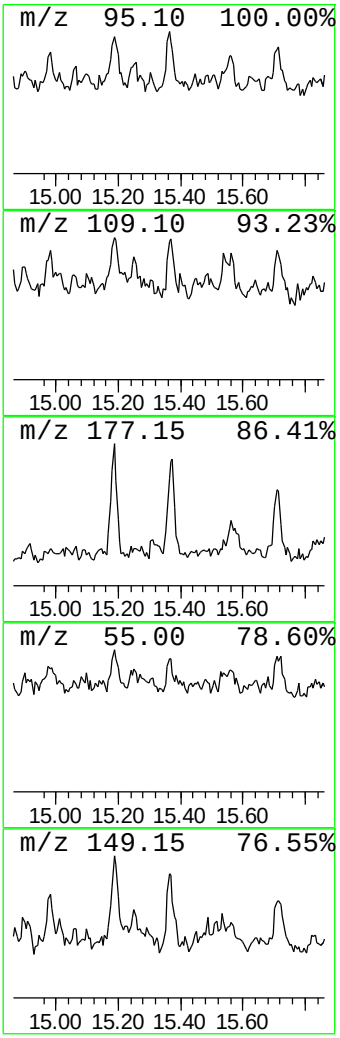
**********

Peak Number 6 17.alfa.,21.beta.-28,30-Bis... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.36 | 8.44 ng | 207527 | Perylene-d12 | 15.22 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 17.alfa.,21.beta.-28,30-Bisnorho... | 384 | C28H48 | 1000360-26-1 | 56 |
| 2 | 5-(1-Isopropenyl-4,5-dimethylbic... | 332 | C22H36O2 | 1000195-69-8 | 49 |
| 3 | 2,6,10,14-Hexadecatetraen-1-ol, ... | 332 | C22H36O2 | 061691-98-3 | 44 |
| 4 | Spiro[4.5]dec-6-en-8-one, 1,7-di... | 220 | C15H24O | 039510-36-6 | 38 |
| 5 | 7-Tetradecyne | 194 | C14H26 | 035216-11-6 | 18 |



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Sample : I4078-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

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**ClientSampleId :** VNJ-211

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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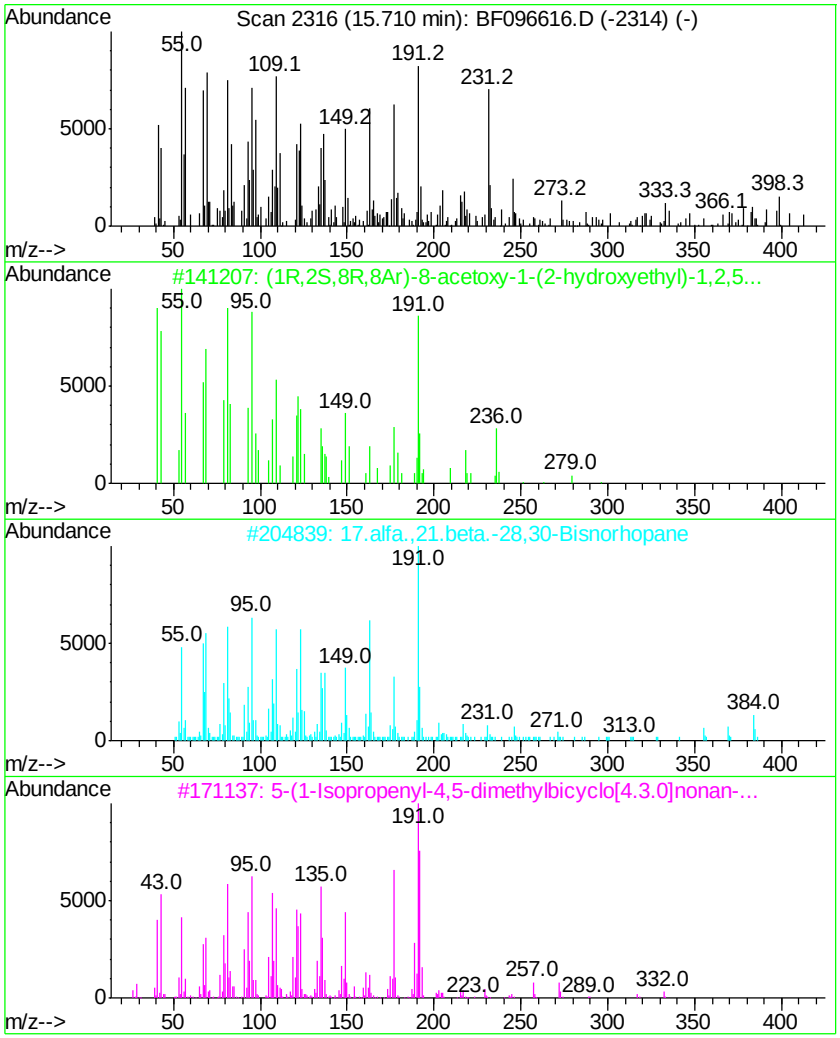
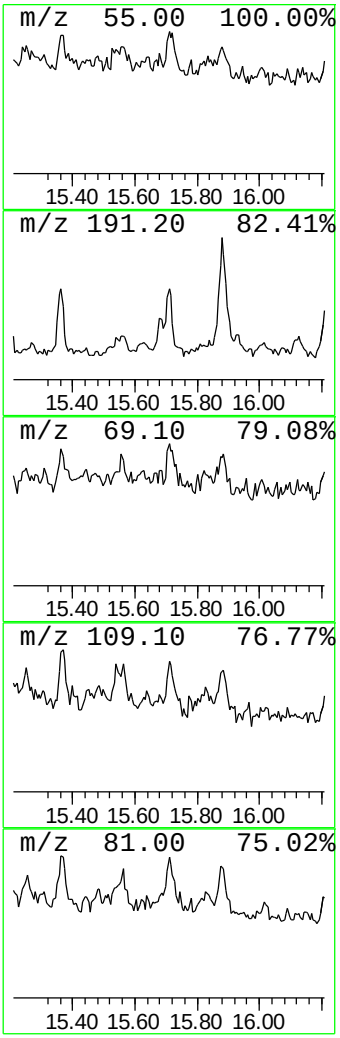
**********

Peak Number 7 (1R,2S,8R,8Ar)-8-acetoxy-1-... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.71 | 12.21 ng | 300214 | Perylene-d12 | 15.22 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (1R,2S,8R,8Ar)-8-acetoxy-1-(2-hy... | 296 | C18H32O3 | 1000298-98-4 | 59 |
| 2 | 17.alfa.,21.beta.-28,30-Bisnorho... | 384 | C28H48 | 1000360-26-1 | 55 |
| 3 | 5-(1-Isopropenyl-4,5-dimethylbic... | 332 | C22H36O2 | 1000195-69-8 | 45 |
| 4 | 28-Nor-17.alpha.(H)-hopane | 398 | C29H50 | 053584-60-4 | 42 |
| 5 | 23,28-Bisnor-17.alpha.(H)-hopane | 384 | C28H48 | 1000101-35-1 | 38 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071017\
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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... | 4.87 | 16.1 | ng | 614370 | 1 | 6.68 | 762665 | 20.0 |
| unknown6.45 | 6.45 | 78.0 | ng | 2973590 | 1 | 6.68 | 762665 | 20.0 |
| Tetradecane | 10.63 | 2.3 | ng | 77862 | 4 | 11.19 | 680173 | 20.0 |
| 1-Nonadecene | 13.68 | 5.2 | ng | 165874 | 5 | 13.82 | 639509 | 20.0 |
| 17.alfa.,21.beta.... | 15.36 | 8.4 | ng | 207527 | 6 | 15.22 | 491722 | 20.0 |
| (1R,2S,8R,8Ar)-8-... | 15.71 | 12.2 | ng | 300214 | 6 | 15.22 | 491722 | 20.0 |