LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111519\
Data File : BP001057.D
Acq On : 15 Nov 2019 23:56
Operator : JU
Sample : K5832-17
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 5-(6-8)

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_P\METHODS\8270-BP110619.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 | 2.346 | 37 | 44 | 52 | rVB | 482971 | 723160 | 9.32% | 1.244% |
| 2 | 5.746 | 616 | 622 | 639 | rVB | 507135 | 831138 | 10.71% | 1.430% |
| 3 | 6.311 | 705 | 718 | 722 | rBV | 3323830 | 4314774 | 55.59% | 7.421% |
| 4 | 7.822 | 966 | 975 | 981 | rVB | 3345701 | 4958482 | 63.88% | 8.528% |
| 5 | 8.010 | 1000 | 1007 | 1011 | rBV | 4098758 | 5170581 | 66.62% | 8.893% |
| 6 | 8.369 | 1062 | 1068 | 1073 | rBV | 1031161 | 1187134 | 15.29% | 2.042% |
| 7 | 8.610 | 1103 | 1109 | 1113 | rBV | 3754473 | 4383230 | 56.47% | 7.539% |
| 8 | 9.246 | 1209 | 1217 | 1221 | rBV | 2486198 | 3182567 | 41.00% | 5.474% |
| 9 | 10.393 | 1406 | 1412 | 1417 | rBV | 1246176 | 1484082 | 19.12% | 2.553% |
| 10 | 12.175 | 1707 | 1715 | 1719 | rBV | 5433707 | 6934983 | 89.35% | 11.928% |
| 11 | 12.840 | 1822 | 1828 | 1832 | rVB | 747211 | 852379 | 10.98% | 1.466% |
| 12 | 13.251 | 1892 | 1898 | 1904 | rBV | 1498522 | 1887559 | 24.32% | 3.247% |
| 13 | 14.545 | 2111 | 2118 | 2129 | rBV | 3361557 | 4323152 | 55.70% | 7.436% |
| 14 | 15.645 | 2301 | 2305 | 2309 | rBV | 1620755 | 1927713 | 24.84% | 3.316% |
| 15 | 15.681 | 2309 | 2311 | 2316 | rVB | 221443 | 215795 | 2.78% | 0.371% |
| 16 | 15.787 | 2326 | 2329 | 2335 | rVB | 74724 | 86563 | 1.12% | 0.149% |
| 17 | 16.439 | 2436 | 2440 | 2445 | rVB | 99302 | 113233 | 1.46% | 0.195% |
| 18 | 16.528 | 2448 | 2455 | 2457 | rBV2 | 191890 | 243327 | 3.13% | 0.419% |
| 19 | 16.551 | 2457 | 2459 | 2463 | rVB | 91029 | 88677 | 1.14% | 0.153% |
| 20 | 16.839 | 2503 | 2508 | 2515 | rVB2 | 54617 | 100668 | 1.30% | 0.173% |
| 21 | 17.386 | 2597 | 2601 | 2605 | rVB | 421820 | 457583 | 5.90% | 0.787% |
| 22 | 17.692 | 2648 | 2653 | 2657 | rVB | 500829 | 578978 | 7.46% | 0.996% |
| 23 | 17.928 | 2686 | 2693 | 2697 | rBV | 7168571 | 7761655 | 100.00% | 13.350% |
| 24 | 18.280 | 2750 | 2753 | 2758 | rBV3 | 86451 | 122362 | 1.58% | 0.210% |
| 25 | 19.157 | 2898 | 2902 | 2914 | rBV2 | 322177 | 628915 | 8.10% | 1.082% |
| 26 | 19.280 | 2917 | 2923 | 2927 | rVV | 1758655 | 2233528 | 28.78% | 3.842% |
| 27 | 19.316 | 2927 | 2929 | 2932 | rVB2 | 273681 | 258499 | 3.33% | 0.445% |
| 28 | 20.569 | 3138 | 3142 | 3146 | rBV | 251186 | 439975 | 5.67% | 0.757% |
| 29 | 20.733 | 3168 | 3170 | 3174 | rVB | 80910 | 92126 | 1.19% | 0.158% |
| 30 | 20.916 | 3197 | 3201 | 3208 | rVB | 163795 | 227132 | 2.93% | 0.391% |
| 31 | 20.986 | 3209 | 3213 | 3217 | rVB | 137851 | 179725 | 2.32% | 0.309% |
| 32 | 21.063 | 3220 | 3226 | 3231 | rBV | 1374753 | 1864639 | 24.02% | 3.207% |
| 33 | 21.180 | 3244 | 3246 | 3252 | rVB2 | 100991 | 130146 | 1.68% | 0.224% |
| 34 | 22.710 | 3503 | 3506 | 3515 | rVB3 | 69912 | 156126 | 2.01% | 0.269% |

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111519\
Data File : BP001057.D
Acq On : 15 Nov 2019 23:56
Operator : JU
Sample : K5832-17
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
5-(6-8)

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_P\METHODS\8270-BP110619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

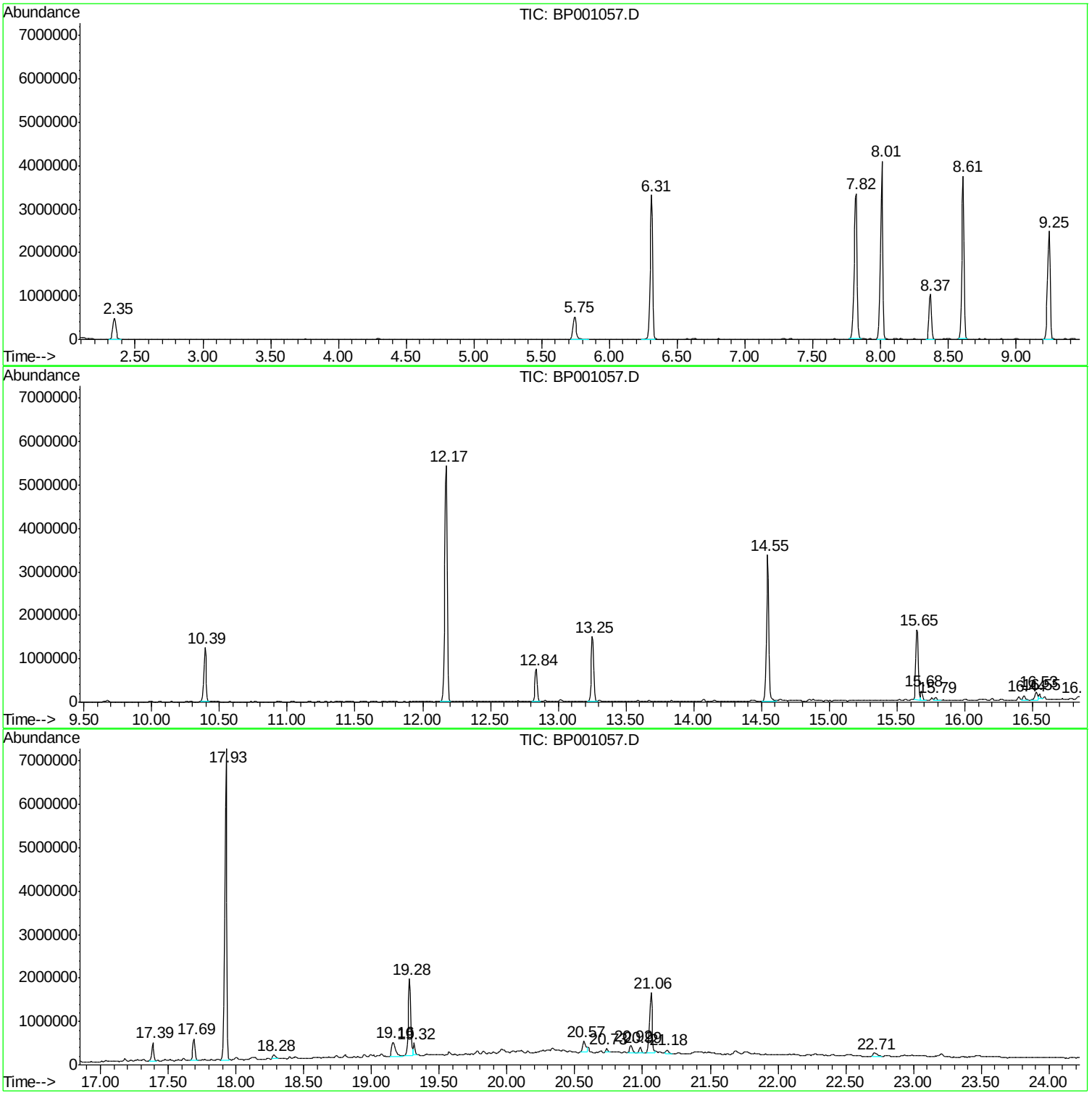
Sum of corrected areas: 58140586

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111519\
Data File : BP001057.D
Acq On : 15 Nov 2019 23:56
Operator : JU
Sample : K5832-17
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
5-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.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 P\DATA\BP111519\
Data File : BP001057.D
Acq On : 15 Nov 2019 23:56
Operator : JU
Sample : K5832-17
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 5-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

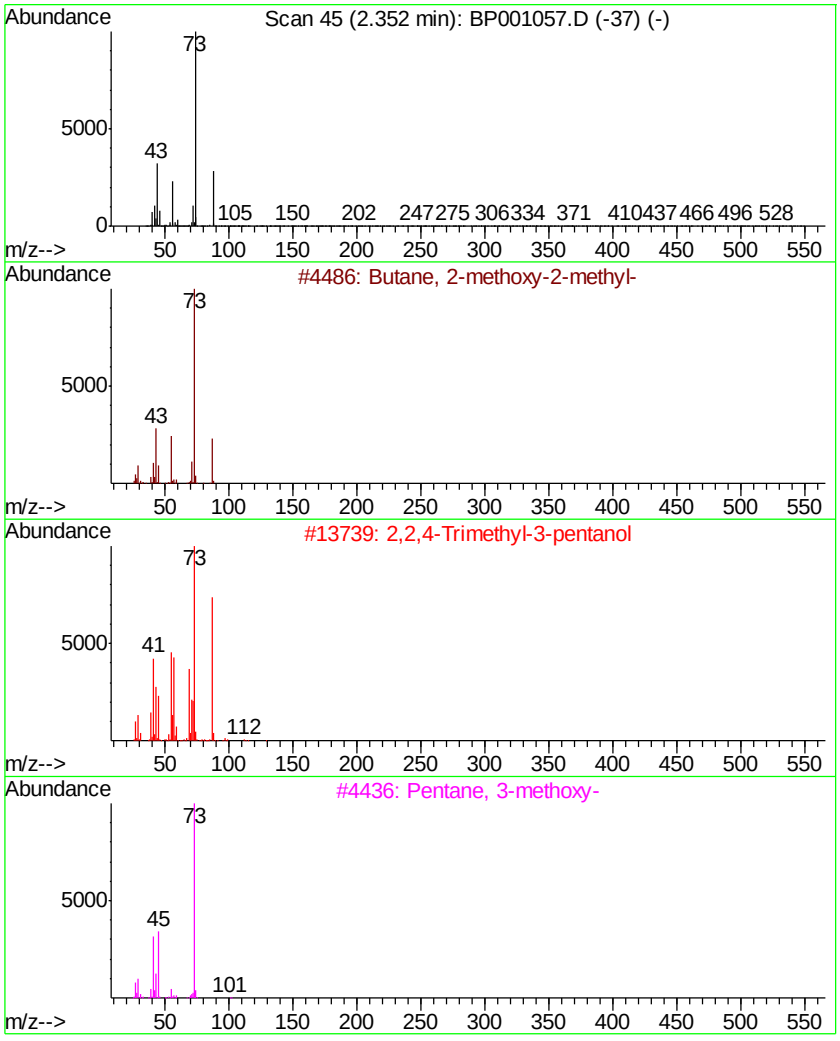
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

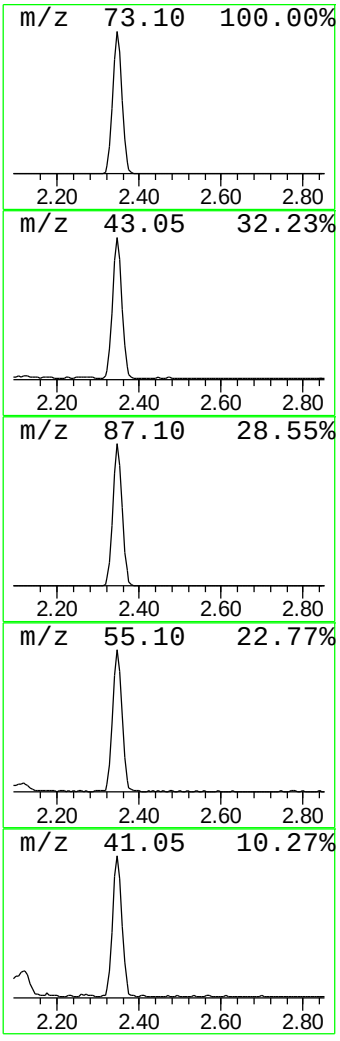
**********

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.35 | 12.18 ng | 723160 | 1,4-Dichlorobenzene-d4 | 8.37 |

| 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 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 23 |
| 4 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |
| 5 | Acetamide, N-ethyl- | 87 | C4H9NO | 000625-50-3 | 9 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111519\
Data File : BP001057.D
Acq On : 15 Nov 2019 23:56
Operator : JU
Sample : K5832-17
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 5-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

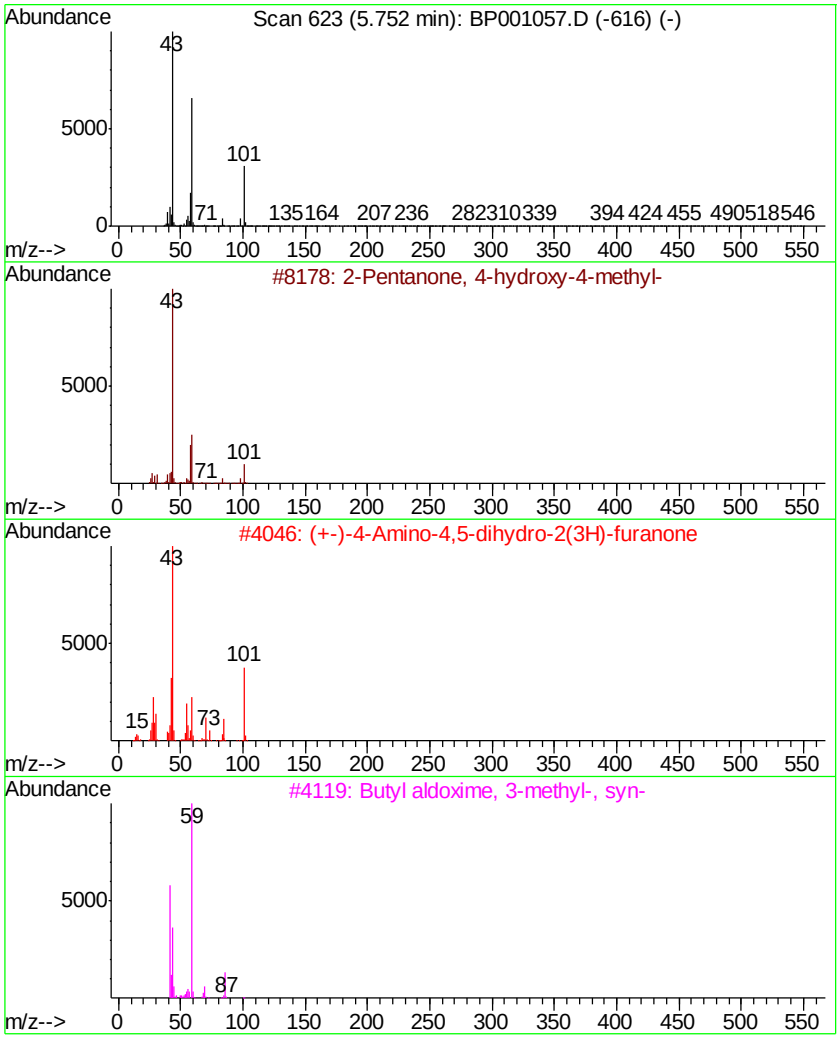
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

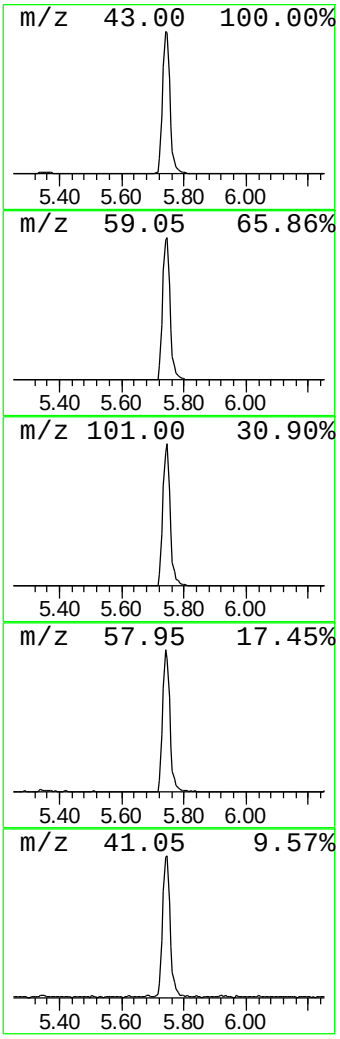
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.75 | 14.00 ng | 831138 | 1,4-Dichlorobenzene-d4 | 8.37 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 64 |
| 2 | (+-)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 47 |
| 3 | Butyl aldoxime, 3-methyl-, syn- | 101 | C5H11NO | 005780-40-5 | 12 |
| 4 | Acetone | 58 | C3H6O | 000067-64-1 | 10 |
| 5 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111519\
Data File : BP001057.D
Acq On : 15 Nov 2019 23:56
Operator : JU
Sample : K5832-17
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 5-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

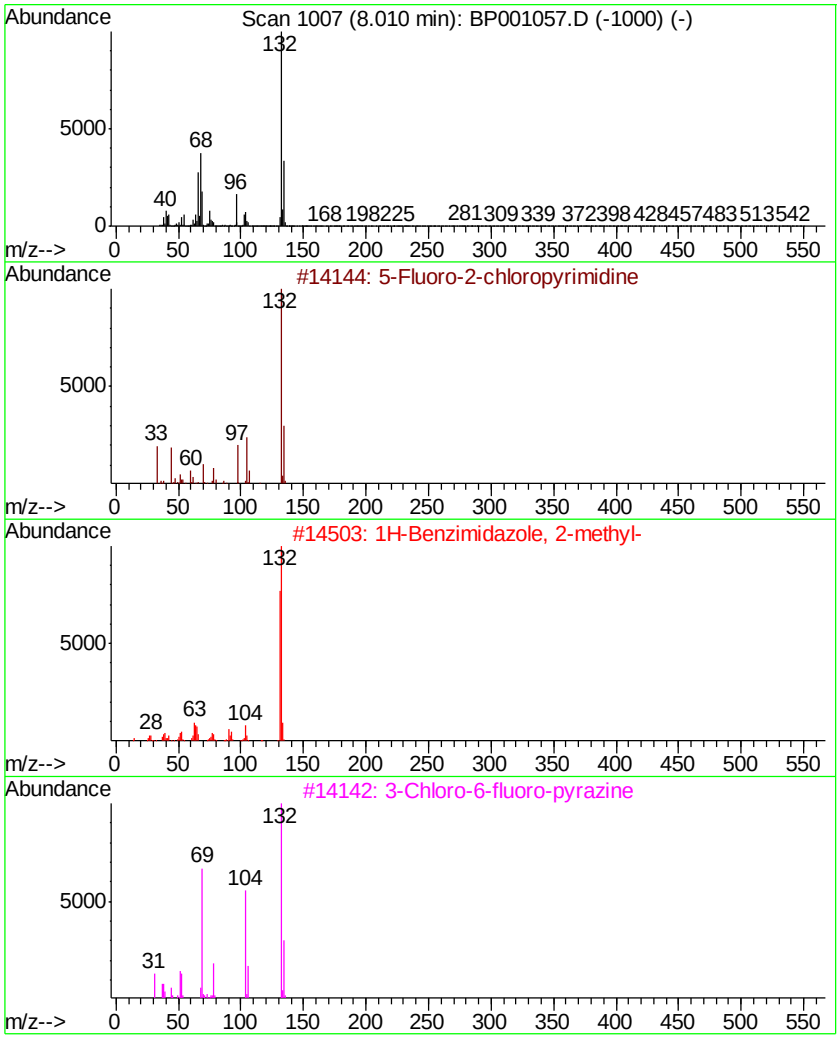
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

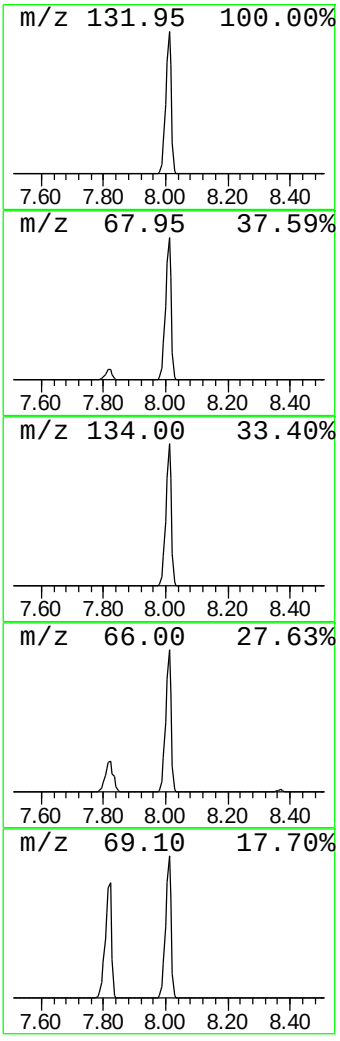
**********

Peak Number 3 unknown8.01 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.01 | 87.11 ng | 5170580 | 1,4-Dichlorobenzene-d4 | 8.37 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 35 |
| 2 | 1H-Benzimidazole, 2-methyl- | 132 | C8H8N2 | 000615-15-6 | 27 |
| 3 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 25 |
| 4 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 17 |
| 5 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 16 |



# Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111519\
Data File : BP001057.D
Acq On : 15 Nov 2019 23:56
Operator : JU
Sample : K5832-17
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 5-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

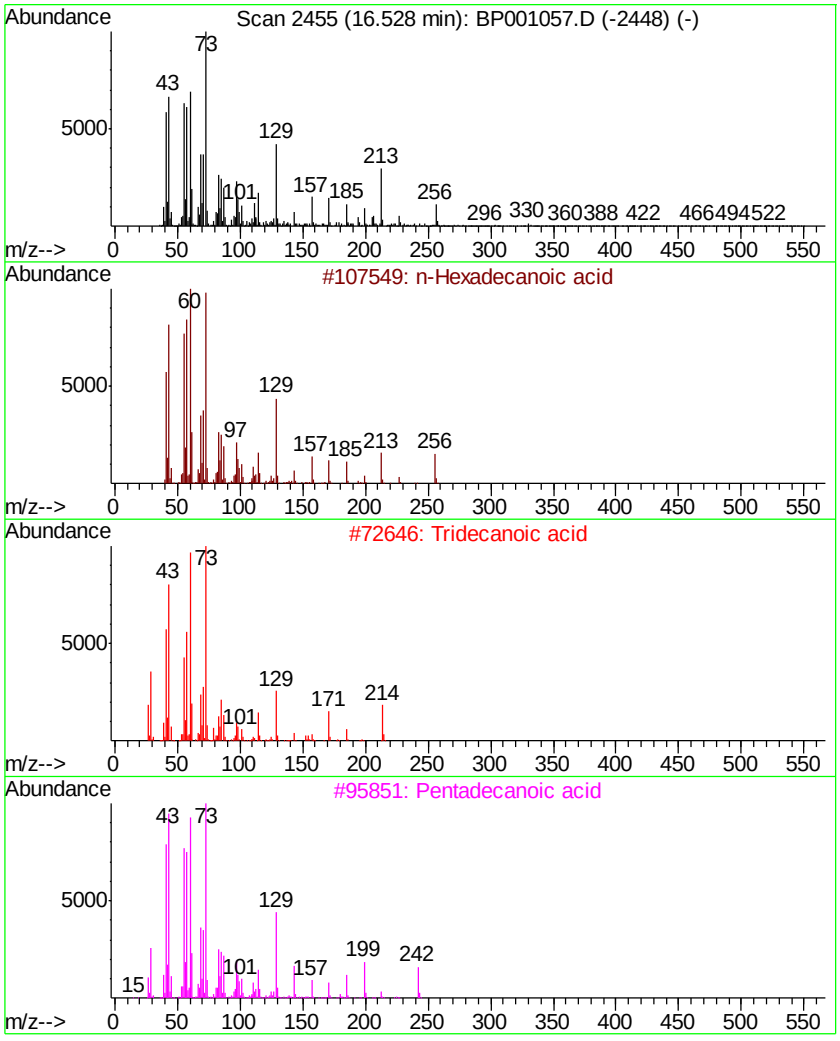
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

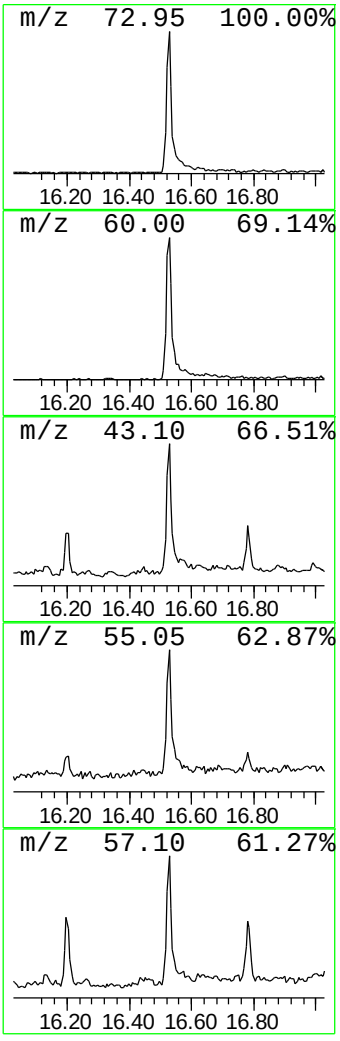
**********

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.53 | 2.52 ng | 243327 | Phenanthrene-d10 | 15.65 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 90 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 81 |
| 4 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 81 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 59 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111519\
Data File : BP001057.D
Acq On : 15 Nov 2019 23:56
Operator : JU
Sample : K5832-17
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 5-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

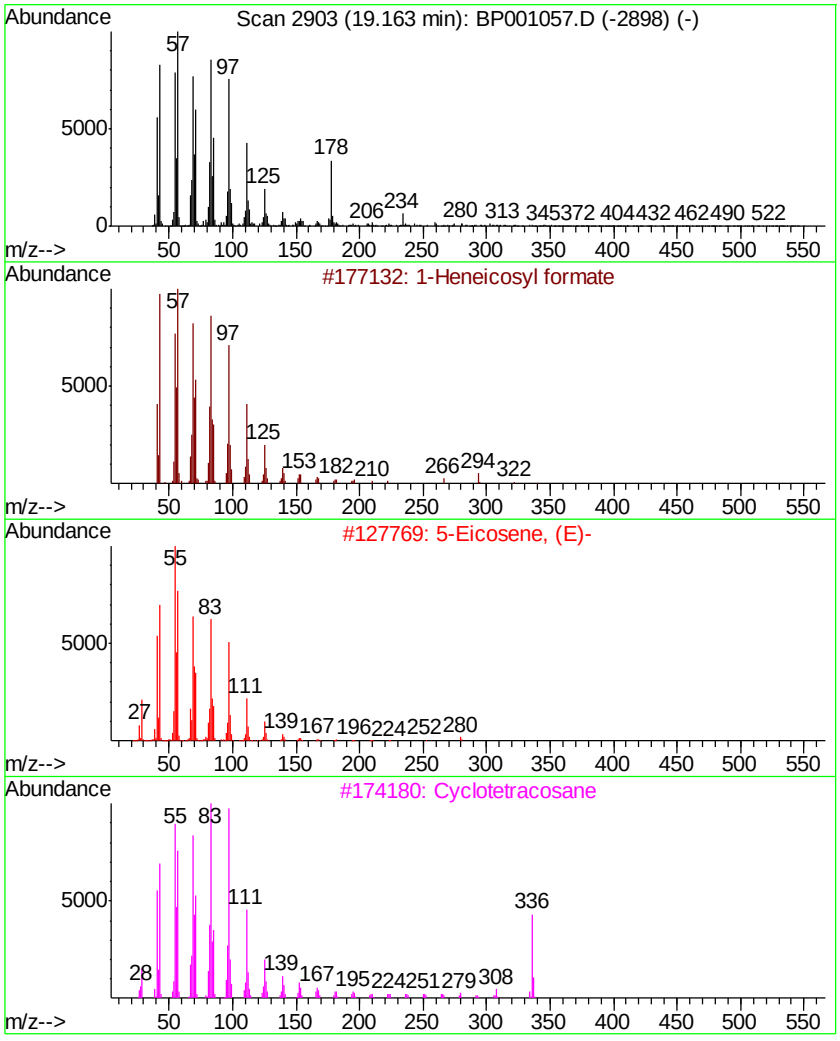
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

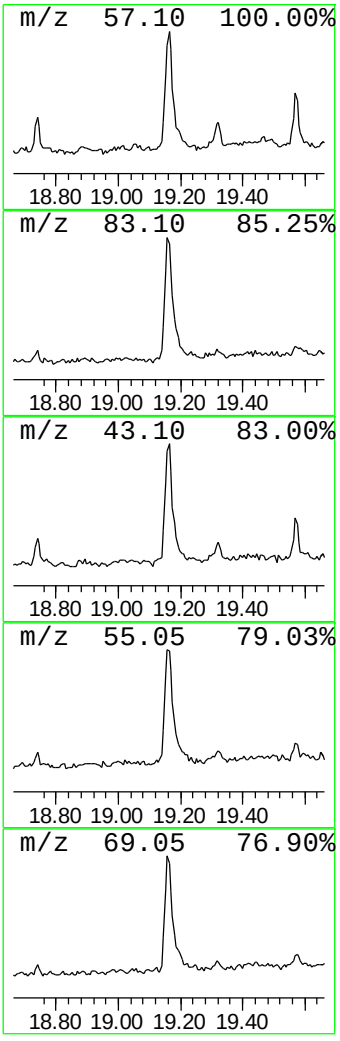
**********

Peak Number 6 1-Heneicosyl formate Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.16 | 5.63 ng | 628915 | Chrysene-d12 | 19.28 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Heneicosyl formate | 340 | C22H44O2 | 077899-03-7 | 99 |
| 2 | 5-Eicosene, (E)- | 280 | C20H40 | 074685-30-6 | 99 |
| 3 | Cyclotetracosane | 336 | C24H48 | 000297-03-0 | 97 |
| 4 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 93 |
| 5 | Cyclopentadecane | 210 | C15H30 | 000295-48-7 | 93 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111519\
Data File : BP001057.D
Acq On : 15 Nov 2019 23:56
Operator : JU
Sample : K5832-17
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 5-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

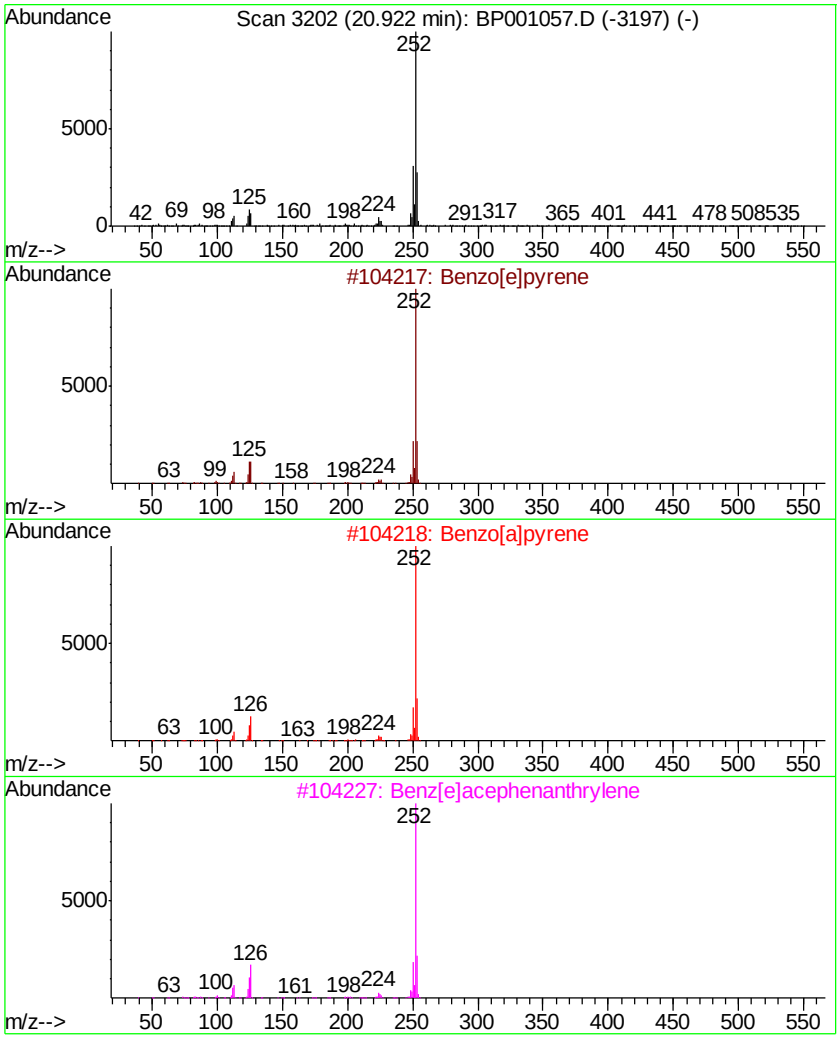
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

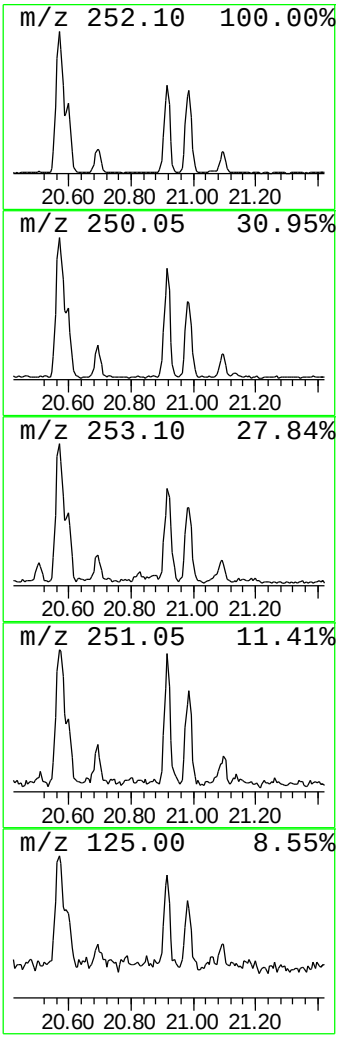
**********

Peak Number 7 Benzo[e]pyrene Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 20.92 | 2.44 ng | 227132 | Perylene-d12 | 21.06 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzo[e]pyrene | 252 | C20H12 | 000192-97-2 | 97 |
| 2 | Benzo[a]pyrene | 252 | C20H12 | 000050-32-8 | 91 |
| 3 | Benz[e]acephenanthrylene | 252 | C20H12 | 000205-99-2 | 91 |
| 4 | Perylene | 252 | C20H12 | 000198-55-0 | 90 |
| 5 | Benzo[k]fluoranthene | 252 | C20H12 | 000207-08-9 | 86 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP111519\
Data File : BP001057.D
Acq On : 15 Nov 2019 23:56
Operator : JU
Sample : K5832-17
Misc :
ALS Vial : 20 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** 5-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.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... | 2.35 | 12.2 | ng | 723160 | 1 | 8.37 | 1187130 | 20.0 |
| 2-Pentanone, 4-hy... | 5.75 | 14.0 | ng | 831138 | 1 | 8.37 | 1187130 | 20.0 |
| unknown8.01 | 8.01 | 87.1 | ng | 5170580 | 1 | 8.37 | 1187130 | 20.0 |
| n-Hexadecanoic acid | 16.53 | 2.5 | ng | 243327 | 4 | 15.65 | 1927710 | 20.0 |
| 1-Heneicosyl formate | 19.16 | 5.6 | ng | 628915 | 5 | 19.28 | 2233530 | 20.0 |
| Benzo[e]pyrene | 20.92 | 2.4 | ng | 227132 | 6 | 21.06 | 1864640 | 20.0 |