LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP090419\
Data File : BP000067.D
Acq On : 04 Sep 2019 15:26
Operator : HP/JU
Sample : K4639-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** SS-01

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-BP083019.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 | 10 | 16 | 23 | rBV | 2109170 | 2609239 | 18.13% | 2.367% |
| 2 | 5.516 | 578 | 583 | 586 | rBV | 10242358 | 9148885 | 63.56% | 8.298% |
| 3 | 6.510 | 747 | 752 | 757 | rBV | 9729242 | 9793084 | 68.03% | 8.882% |
| 4 | 6.663 | 773 | 778 | 781 | rBV | 10967875 | 9877774 | 68.62% | 8.959% |
| 5 | 6.716 | 784 | 787 | 799 | rVB | 443528 | 394030 | 2.74% | 0.357% |
| 6 | 6.893 | 814 | 817 | 820 | rVB | 3547042 | 2600448 | 18.07% | 2.359% |
| 7 | 7.052 | 840 | 844 | 847 | rBV | 10392508 | 8190171 | 56.90% | 7.428% |
| 8 | 7.446 | 907 | 911 | 914 | rBV | 6748089 | 5920600 | 41.13% | 5.370% |
| 9 | 8.175 | 1031 | 1035 | 1038 | rBV | 4399311 | 3410905 | 23.70% | 3.094% |
| 10 | 9.251 | 1214 | 1218 | 1222 | rBV | 13897178 | 13027420 | 90.50% | 11.816% |
| 11 | 9.375 | 1236 | 1239 | 1242 | rVB | 222294 | 200196 | 1.39% | 0.182% |
| 12 | 9.646 | 1281 | 1285 | 1288 | rBV | 1658814 | 1223800 | 8.50% | 1.110% |
| 13 | 9.934 | 1331 | 1334 | 1338 | rBV | 4725183 | 4182222 | 29.05% | 3.793% |
| 14 | 10.728 | 1465 | 1469 | 1472 | rBV | 9489065 | 7700762 | 53.50% | 6.984% |
| 15 | 11.434 | 1585 | 1589 | 1592 | rBV | 5352652 | 4405244 | 30.60% | 3.995% |
| 16 | 11.963 | 1675 | 1679 | 1684 | rBV | 532095 | 512897 | 3.56% | 0.465% |
| 17 | 12.698 | 1799 | 1804 | 1811 | rBV | 329451 | 393315 | 2.73% | 0.357% |
| 18 | 12.757 | 1811 | 1814 | 1823 | rVV | 218896 | 229471 | 1.59% | 0.208% |
| 19 | 13.040 | 1857 | 1862 | 1865 | rBV | 14919513 | 14394512 | 100.00% | 13.056% |
| 20 | 13.522 | 1941 | 1944 | 1946 | rBV2 | 150271 | 159729 | 1.11% | 0.145% |
| 21 | 13.945 | 2012 | 2016 | 2033 | rBV | 847816 | 1200611 | 8.34% | 1.089% |
| 22 | 14.098 | 2038 | 2042 | 2046 | rBV | 5080553 | 4232352 | 29.40% | 3.839% |
| 23 | 14.281 | 2069 | 2073 | 2082 | rVB | 168865 | 194097 | 1.35% | 0.176% |
| 24 | 14.586 | 2123 | 2125 | 2137 | rVB | 270361 | 284951 | 1.98% | 0.258% |
| 25 | 14.916 | 2177 | 2181 | 2185 | rVB | 290334 | 301008 | 2.09% | 0.273% |
| 26 | 15.275 | 2238 | 2242 | 2253 | rBV | 330318 | 387142 | 2.69% | 0.351% |
| 27 | 15.622 | 2295 | 2301 | 2308 | rBV | 3539552 | 4244167 | 29.48% | 3.849% |
| 28 | 15.686 | 2308 | 2312 | 2322 | rVB | 281826 | 379145 | 2.63% | 0.344% |
| 29 | 16.157 | 2387 | 2392 | 2396 | rBV | 197881 | 296280 | 2.06% | 0.269% |
| 30 | 16.204 | 2396 | 2400 | 2411 | rVB2 | 101812 | 208296 | 1.45% | 0.189% |
| 31 | 16.704 | 2480 | 2485 | 2494 | rVB2 | 82237 | 153421 | 1.07% | 0.139% |

Sum of corrected areas: 110256174

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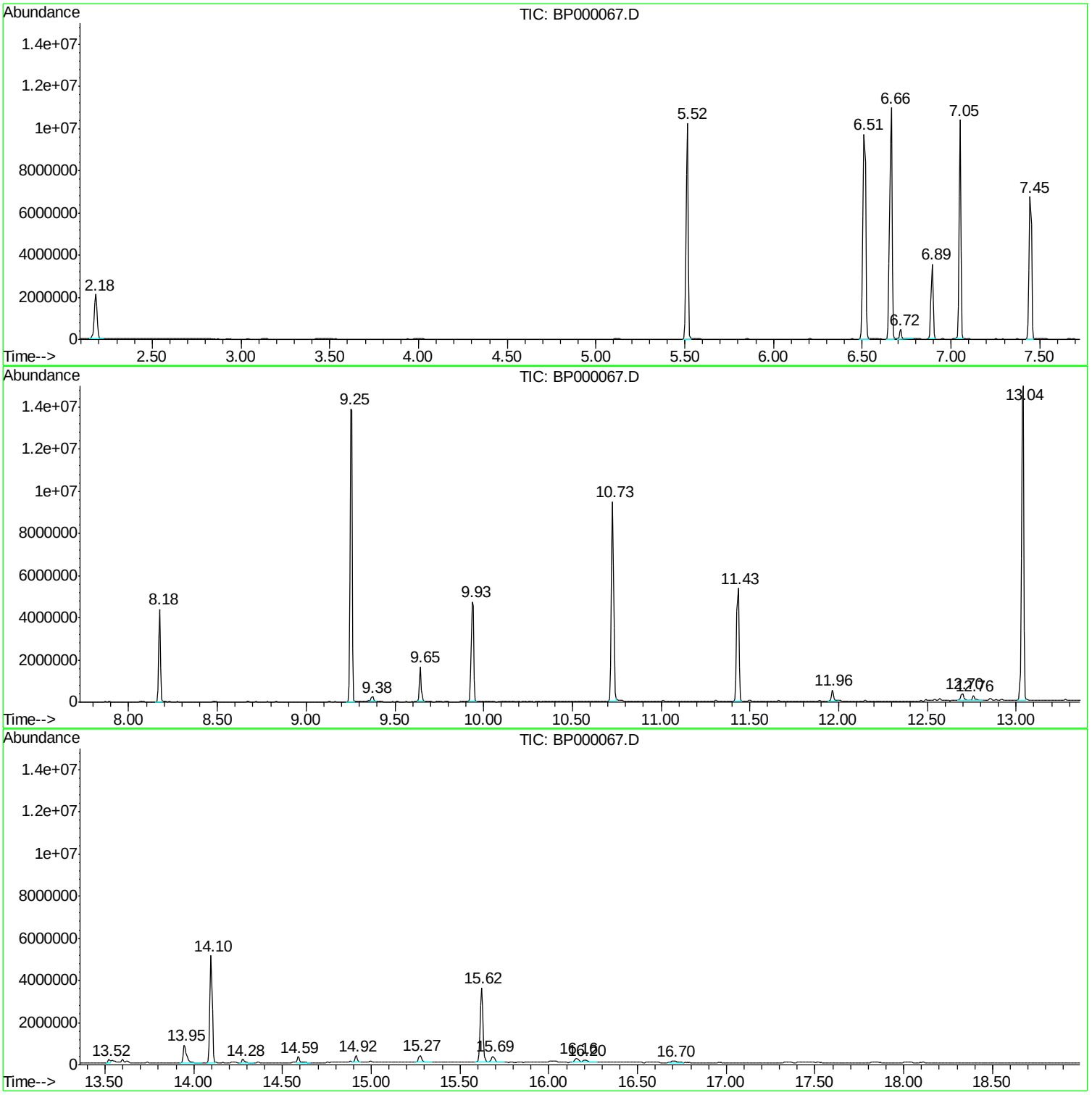
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :**
BNA_P
**ClientSampleId :**
SS-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP083019.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

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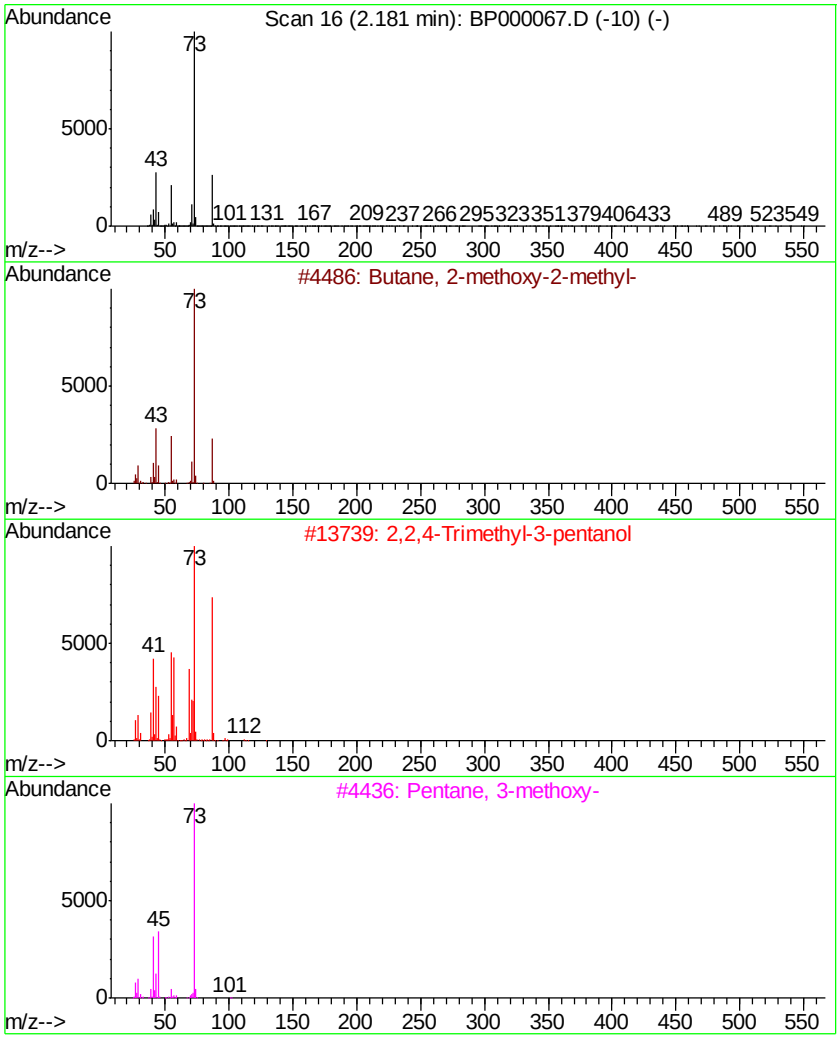
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

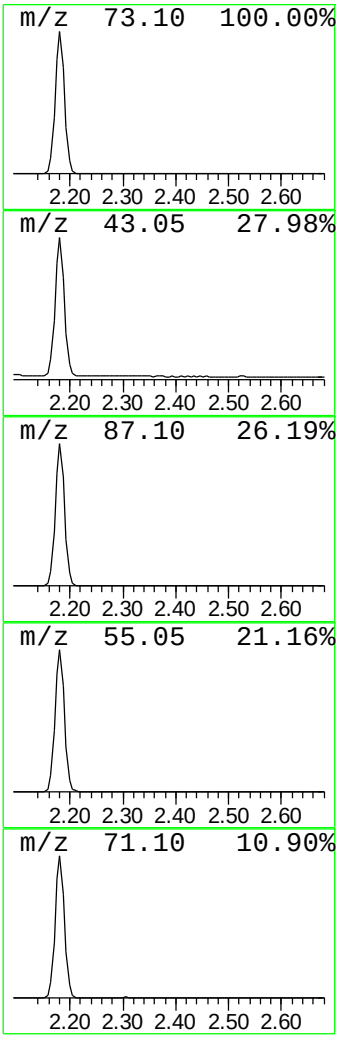
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.18 | 20.07 ng | 2609240 | 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 | 40 |
| 3 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 17 |
| 4 | Acetamide, N-ethyl- | 87 | C4H9NO | 000625-50-3 | 9 |
| 5 | Borane, dimethoxy- | 74 | C2H7BO2 | 004542-61-4 | 9 |



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Sample : K4639-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** SS-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

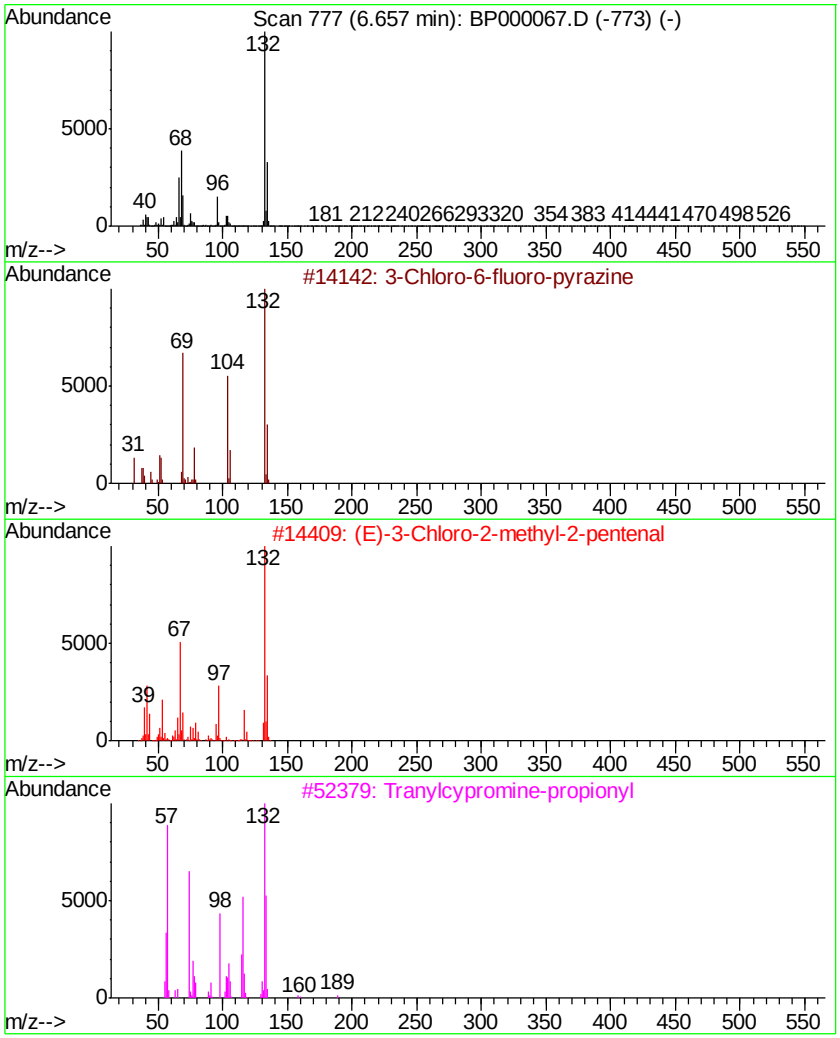
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

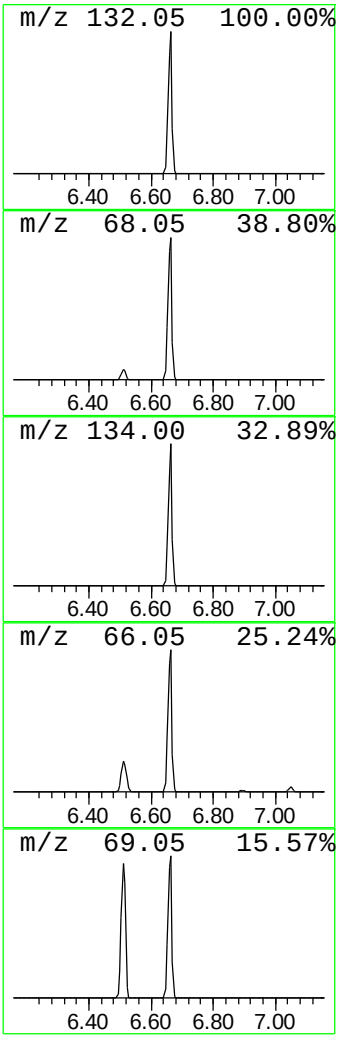
**********

Peak Number 2 unknown6.66 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.66 | 75.97 ng | 9877770 | 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 | 38 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 17 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 16 |
| 4 | 1,3-Cyclopentanedione, 2-chloro- | 132 | C5H5ClO2 | 014203-19-1 | 9 |
| 5 | (5-Methyl-2-pyridyl)acetonitrile | 132 | C8H8N2 | 1000241-93-9 | 9 |



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**Instrument :** BNA_P
**ClientSampleId :** SS-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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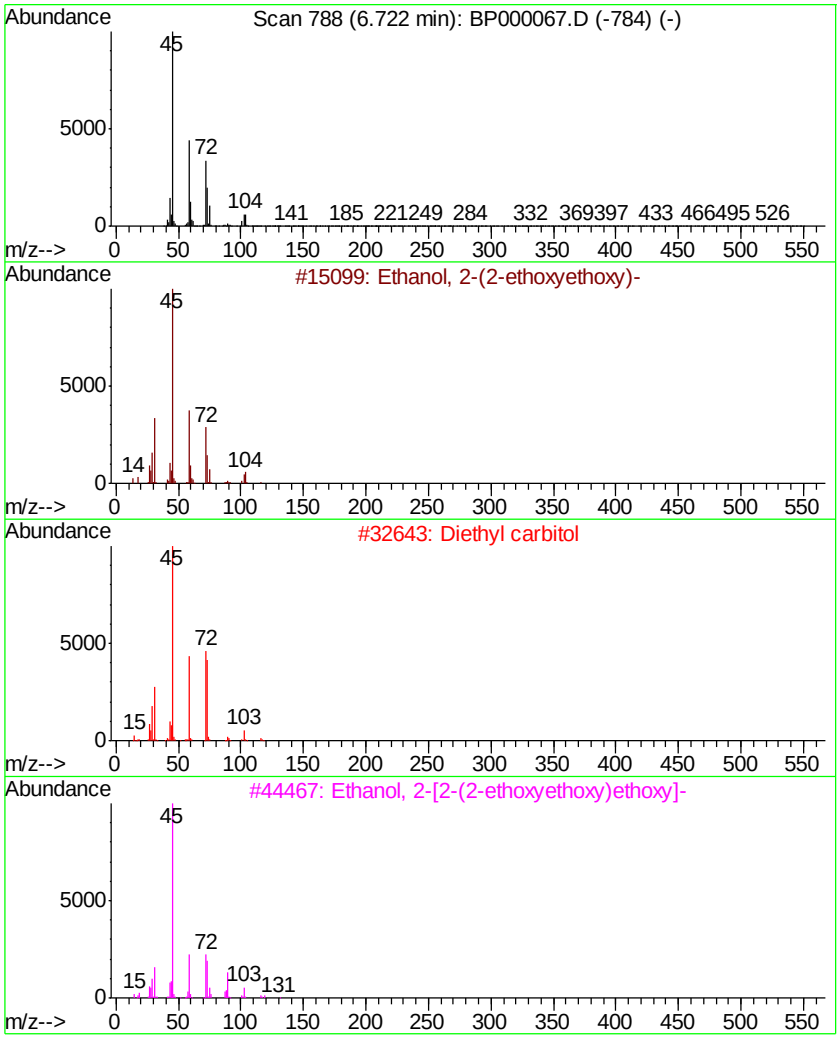
TIC Integration Parameters: LSCINT.P

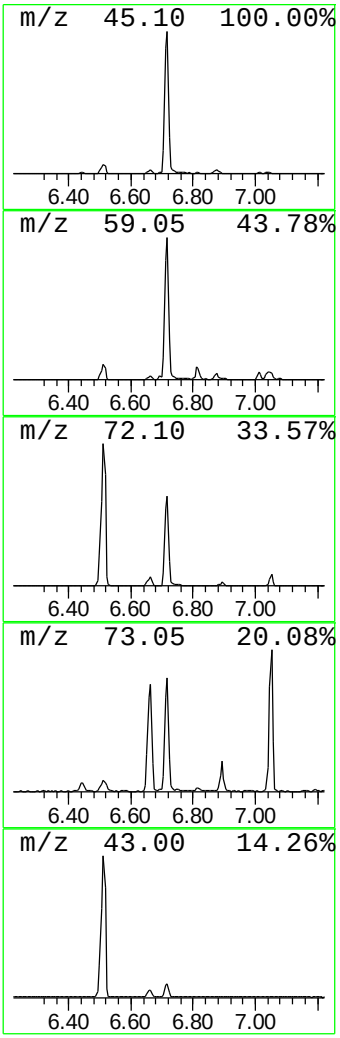
**********

Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.72 | 3.03 ng | 394030 | 1,4-Dichlorobenzene-d4 | 6.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2-(2-ethoxyethoxy)- | 134 | C6H14O3 | 000111-90-0 | 90 |
| 2 | Diethyl carbitol | 162 | C8H18O3 | 000112-36-7 | 72 |
| 3 | Ethanol, 2-[2-(2-ethoxyethoxy)et... | 178 | C8H18O4 | 000112-50-5 | 59 |
| 4 | 2-Propanol, 1-(1-methylethoxy)- | 118 | C6H14O2 | 003944-36-3 | 50 |
| 5 | Ethanol, 2-(2-methoxyethoxy)- | 120 | C5H12O3 | 000111-77-3 | 42 |



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ALS Vial : 17 Sample Multiplier: 1

**Instrument :** BNA_P
**ClientSampleId :** SS-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

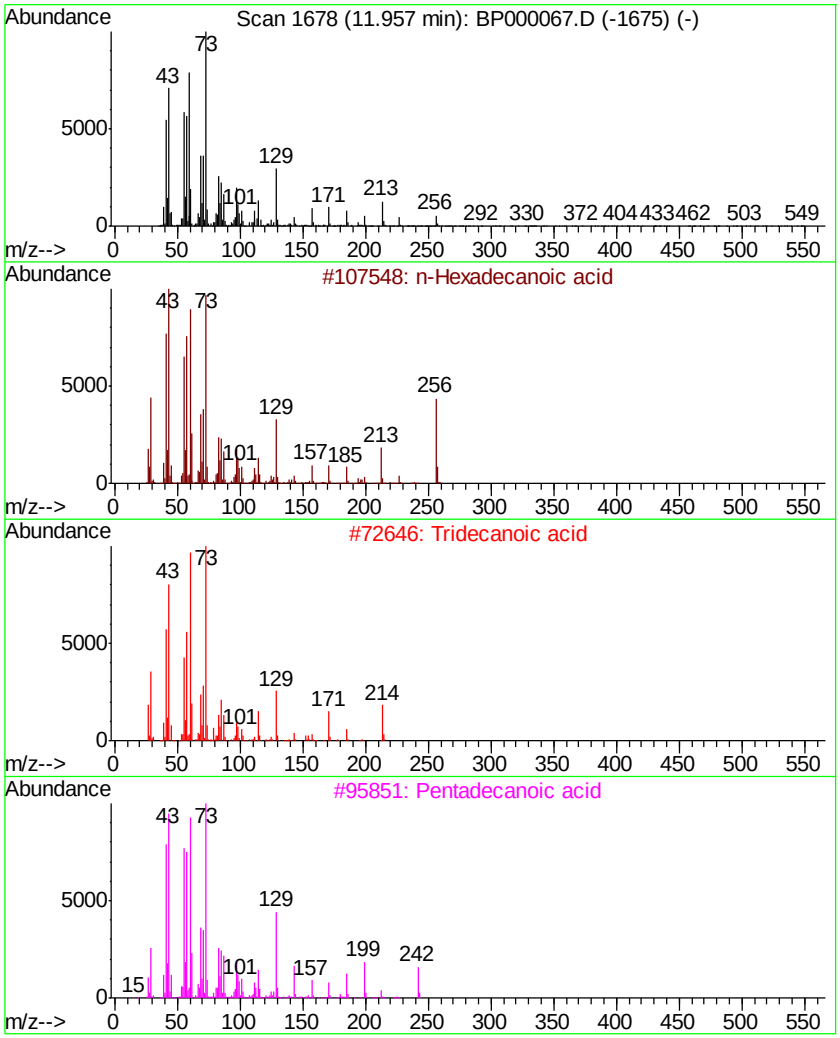
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

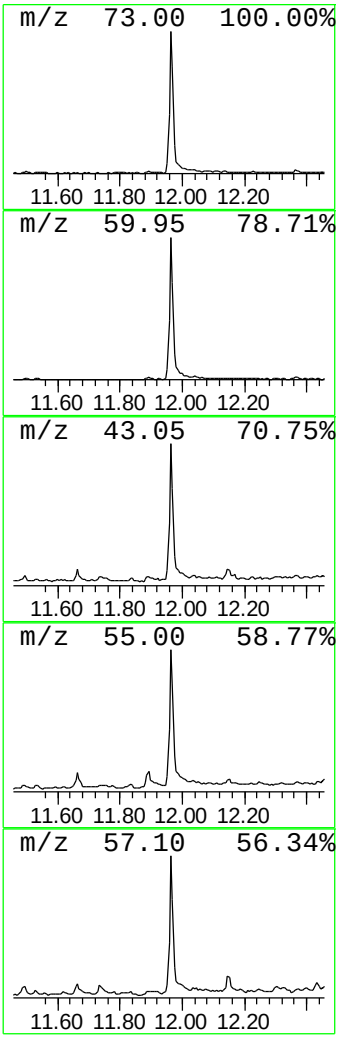
**********

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.96 | 2.33 ng | 512897 | Phenanthrene-d10 | 11.43 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 91 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 90 |
| 4 | Octadecanoic acid | 284 | C18H36O2 | 000057-11-4 | 90 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 72 |



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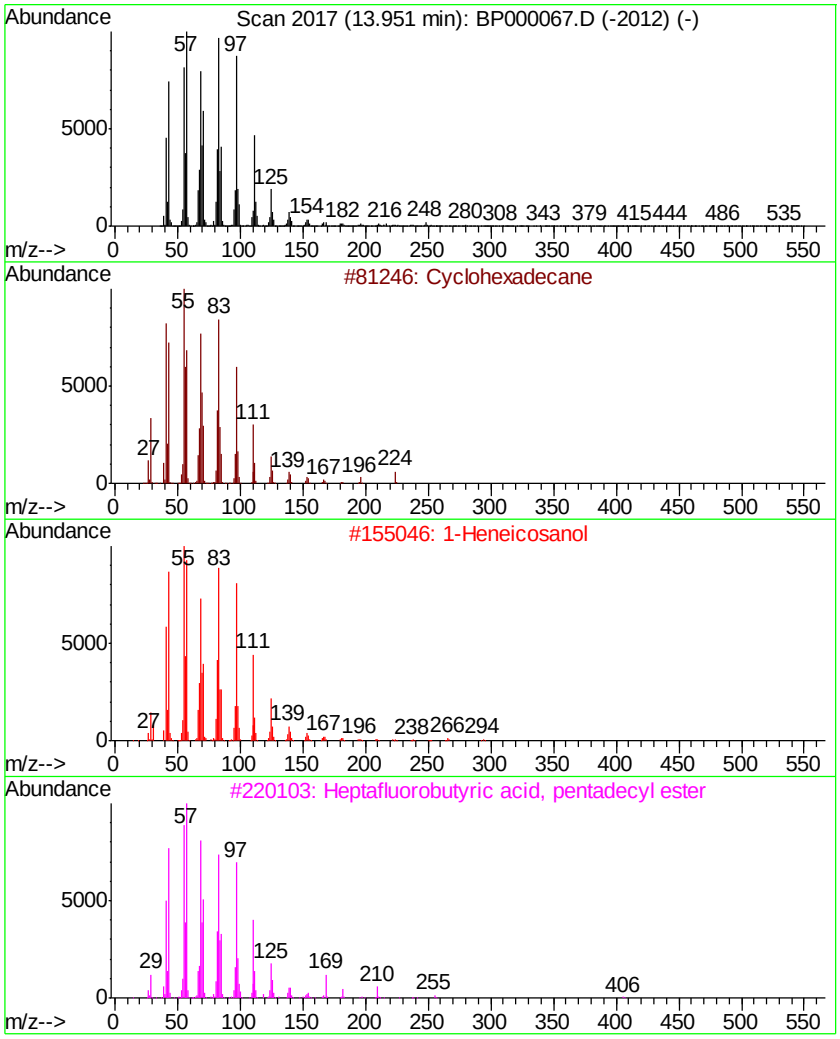
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

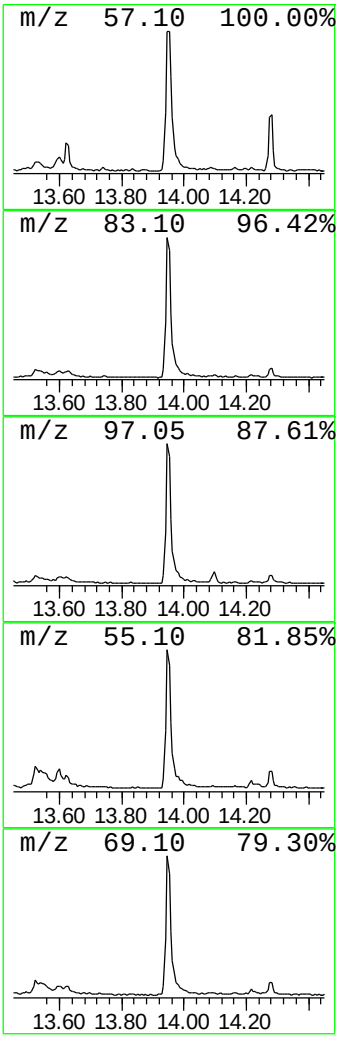
**********

Peak Number 6 Cyclohexadecane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.95 | 5.67 ng | 1200610 | Chrysene-d12 | 14.10 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclohexadecane | 224 | C16H32 | 000295-65-8 | 94 |
| 2 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 94 |
| 3 | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 94 |
| 4 | 1-Heptacosanol | 396 | C27H56O | 002004-39-9 | 94 |
| 5 | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2 | 959010-23-2 | 94 |



Tentatively Identified Compound (LSC) summary

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| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Butane, 2-methoxy... | 2.18 | 20.1 | ng | 2609240 | 1 | 6.89 | 2600450 | 20.0 |
| unknown6.66 | 6.66 | 76.0 | ng | 9877770 | 1 | 6.89 | 2600450 | 20.0 |
| Ethanol, 2-(2-eth... | 6.72 | 3.0 | ng | 394030 | 1 | 6.89 | 2600450 | 20.0 |
| n-Hexadecanoic acid | 11.96 | 2.3 | ng | 512897 | 4 | 11.43 | 4405240 | 20.0 |
| Cyclohexadecane | 13.95 | 5.7 | ng | 1200610 | 5 | 14.10 | 4232350 | 20.0 |