LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124644.D
Acq On : 21 Jul 2021 00:20
Operator : JU/CG
Sample : M3040-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-PS-01-076

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_F\METHODS\8270-BF070721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124644.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.222 | 20 | 23 | 27 | rBB | 8005 | 8706 | 5.70% | 0.899% |
| 2 | 5.134 | 515 | 518 | 521 | rBB | 2291 | 2680 | 1.75% | 0.277% |
| 3 | 5.516 | 579 | 583 | 586 | rBB | 137199 | 132341 | 86.65% | 13.661% |
| 4 | 6.522 | 748 | 754 | 756 | rBB | 137485 | 138386 | 90.61% | 14.285% |
| 5 | 6.904 | 816 | 819 | 821 | rBB | 43885 | 35908 | 23.51% | 3.707% |
| 6 | 7.463 | 909 | 914 | 917 | rBB | 101965 | 91647 | 60.00% | 9.460% |
| 7 | 8.081 | 1016 | 1019 | 1022 | rBB | 19890 | 13252 | 8.68% | 1.368% |
| 8 | 8.186 | 1033 | 1037 | 1040 | rBB | 69218 | 50990 | 33.39% | 5.263% |
| 9 | 9.263 | 1216 | 1220 | 1223 | rBV | 199161 | 152733 | 100.00% | 15.766% |
| 10 | 9.945 | 1332 | 1336 | 1339 | rBB | 67639 | 55560 | 36.38% | 5.735% |
| 11 | 10.727 | 1466 | 1469 | 1472 | rBB | 99404 | 87143 | 57.06% | 8.995% |
| 12 | 11.427 | 1585 | 1588 | 1592 | rBB | 57328 | 44976 | 29.45% | 4.643% |
| 13 | 11.945 | 1674 | 1676 | 1679 | rBB | 10744 | 8079 | 5.29% | 0.834% |
| 14 | 13.016 | 1854 | 1858 | 1861 | rBB | 109964 | 84166 | 55.11% | 8.688% |
| 15 | 13.910 | 2007 | 2010 | 2014 | rBB | 4917 | 5373 | 3.52% | 0.555% |
| 16 | 14.068 | 2033 | 2037 | 2040 | rBB | 28111 | 23272 | 15.24% | 2.402% |
| 17 | 14.545 | 2114 | 2118 | 2121 | rBB | 2736 | 2819 | 1.85% | 0.291% |
| 18 | 15.192 | 2225 | 2228 | 2231 | rBB | 2404 | 2790 | 1.83% | 0.288% |
| 19 | 15.557 | 2285 | 2290 | 2293 | rBB | 19744 | 22364 | 14.64% | 2.309% |
| 20 | 16.086 | 2376 | 2380 | 2385 | rBB | 4174 | 5578 | 3.65% | 0.576% |

Sum of corrected areas: 968763

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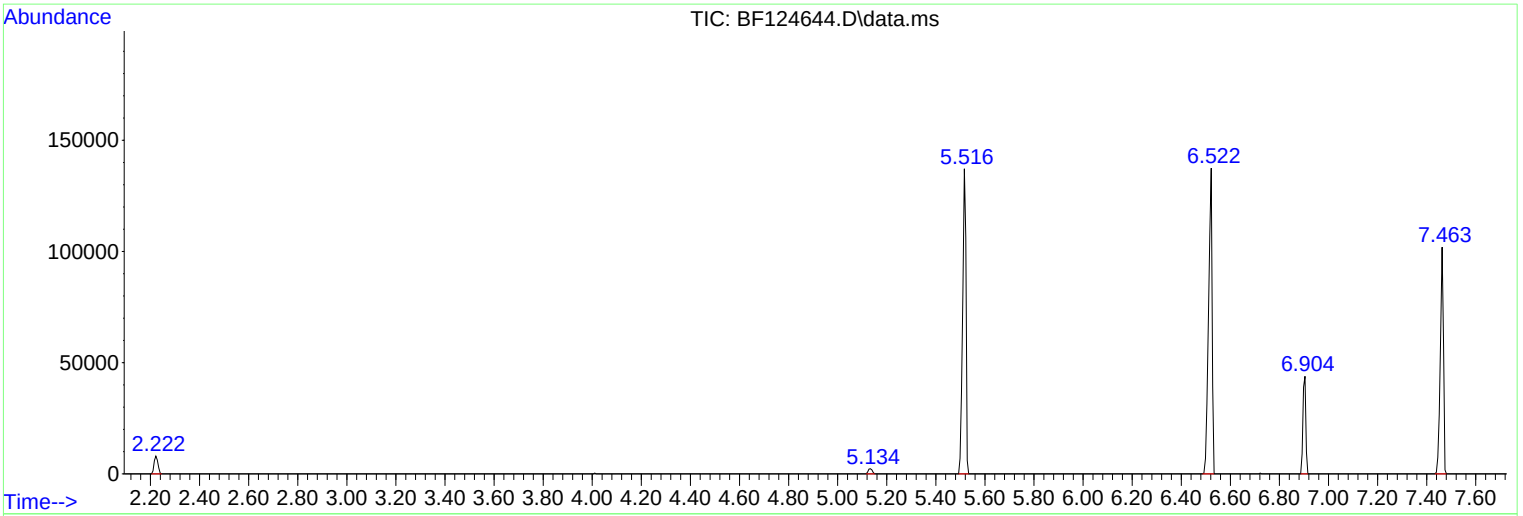
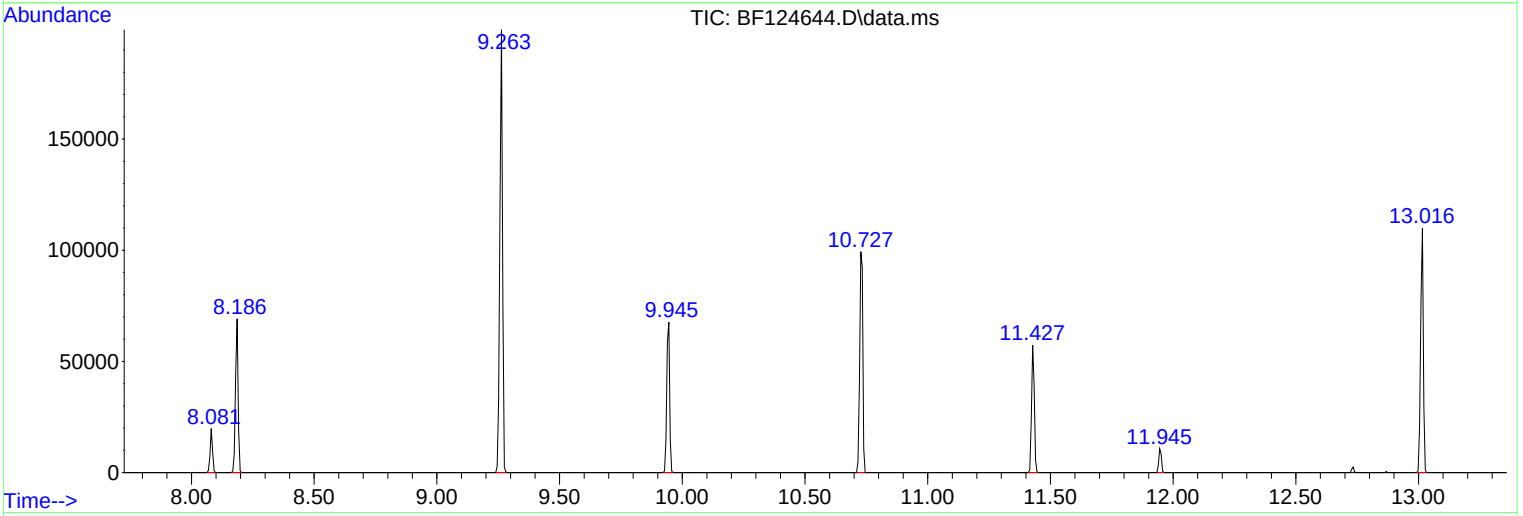
Misc :
ALS Vial : 9 Sample Multiplier: 1

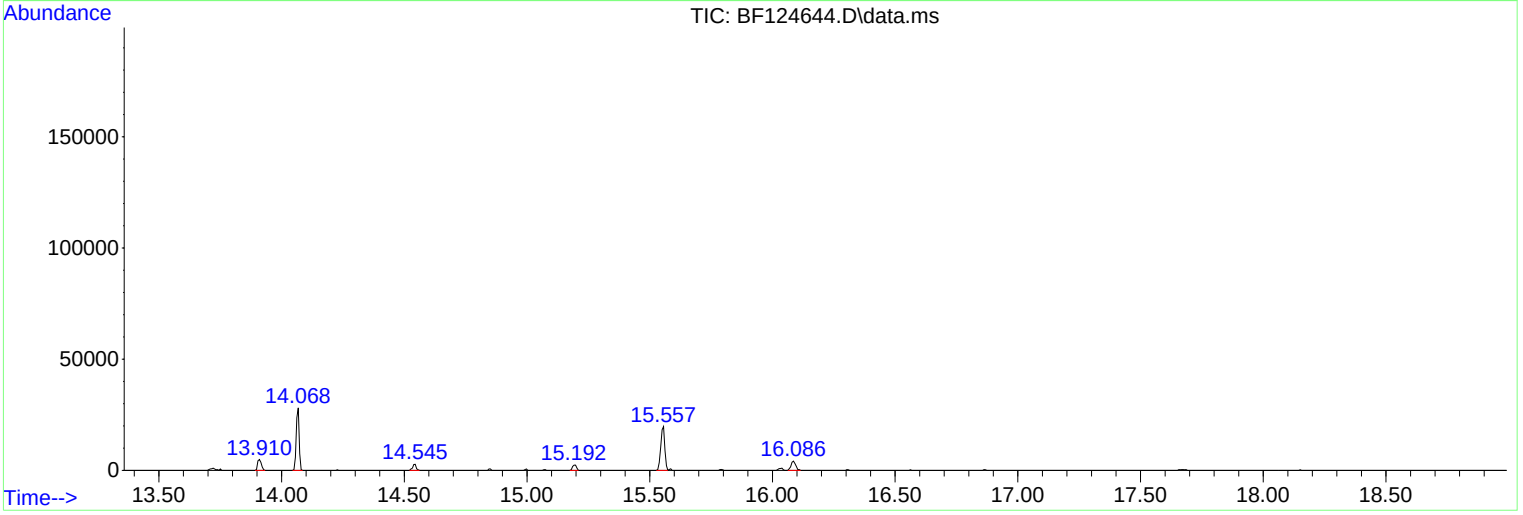
**Instrument :**
BNA_F
**ClientSampleId :**
FK-PS-01-076

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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FK-PS-01-076

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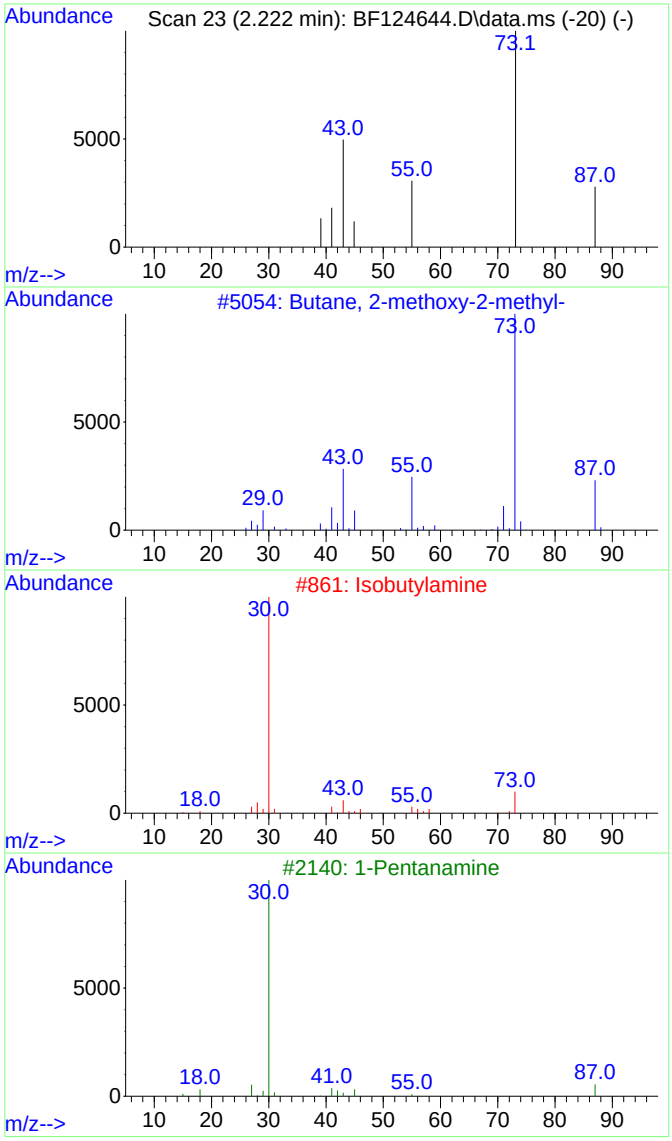
TIC Integration Parameters: LSCINT.P

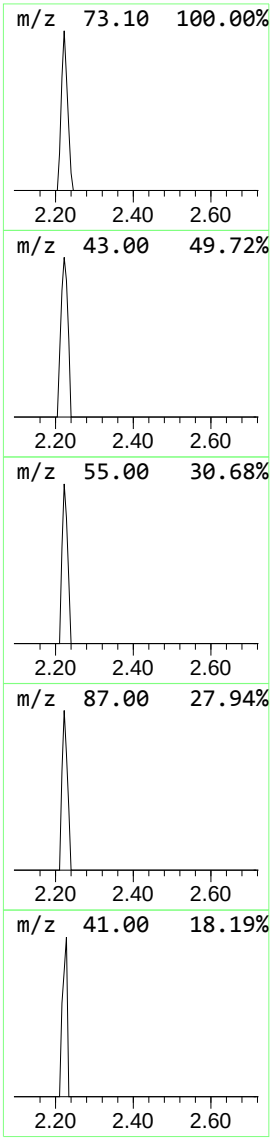
**********

Peak Number 1 unknown2.222 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.222 | 4.85 ng | 8706 | 1,4-Dichlorobenzene-d4 | 6.904 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butane, 2-methoxy-2-methyl- | 102 | C6H14O | 000994-05-8 | 9 |
| 2 | Isobutylamine | 73 | C4H11N | 000078-81-9 | 5 |
| 3 | 1-Pentanamine | 87 | C5H13N | 000110-58-7 | 4 |
| 4 | 1-Butanamine, 3-methyl- | 87 | C5H13N | 000107-85-7 | 4 |
| 5 | 2-Butanone, 3-methoxy-3-methyl- | 116 | C6H12O2 | 036687-98-6 | 4 |



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Data File : BF124644.D
Acq On : 21 Jul 2021 00:20
Operator : JU/CG
Sample : M3040-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-PS-01-076

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

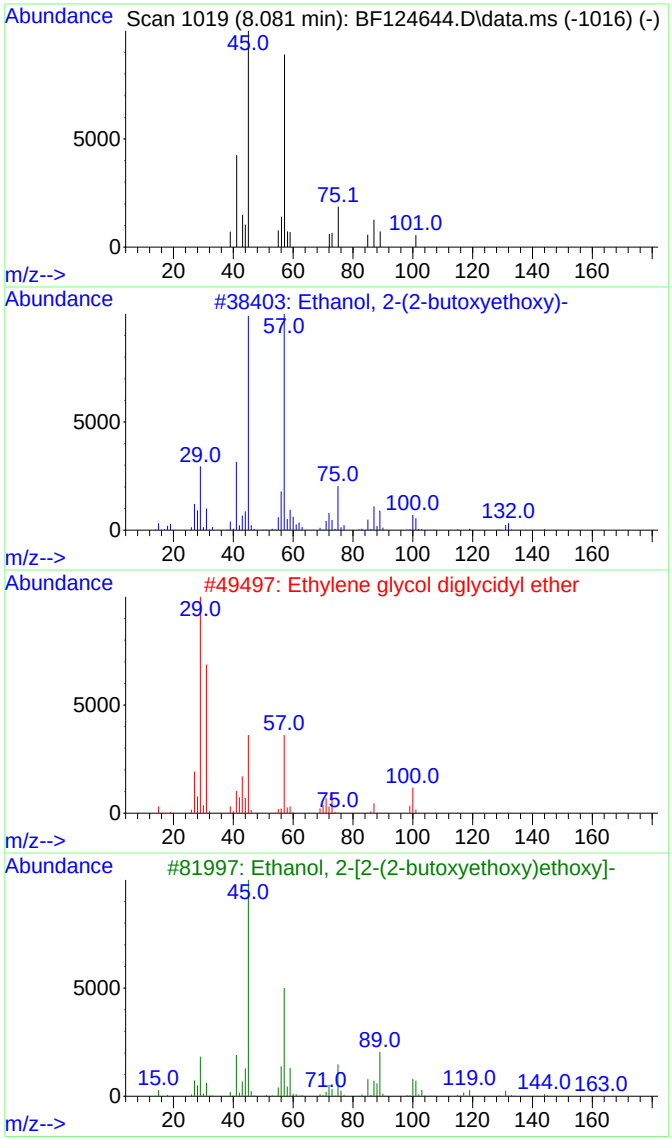
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

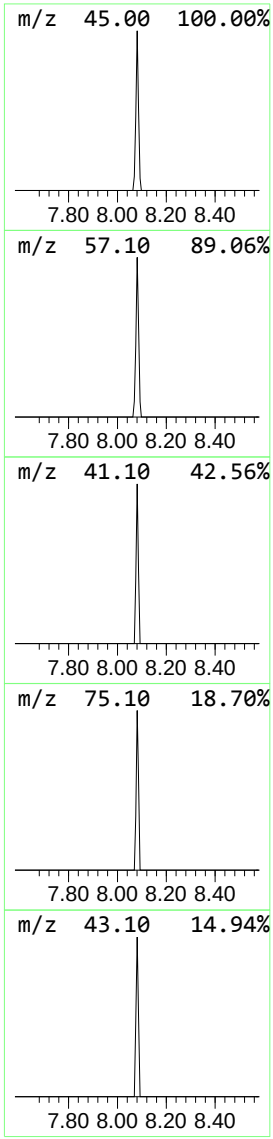
**********

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.081 | 5.20 ng | 13252 | Naphthalene-d8 | 8.186 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2-(2-butoxyethoxy)- | 162 | C8H18O3 | 000112-34-5 | 83 |
| 2 | Ethylene glycol diglycidyl ether | 174 | C8H14O4 | 002224-15-9 | 39 |
| 3 | Ethanol, 2-[2-(2-butoxyethoxy)et... | 206 | C10H22O4 | 000143-22-6 | 38 |
| 4 | Sulfurous acid, isobutyl 2-methy... | 238 | C10H22O4S | 1000309-20-3 | 33 |
| 5 | Ethylene glycol monoisobutyl ether | 118 | C6H14O2 | 004439-24-1 | 33 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124644.D
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Operator : JU/CG
Sample : M3040-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
FK-PS-01-076

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
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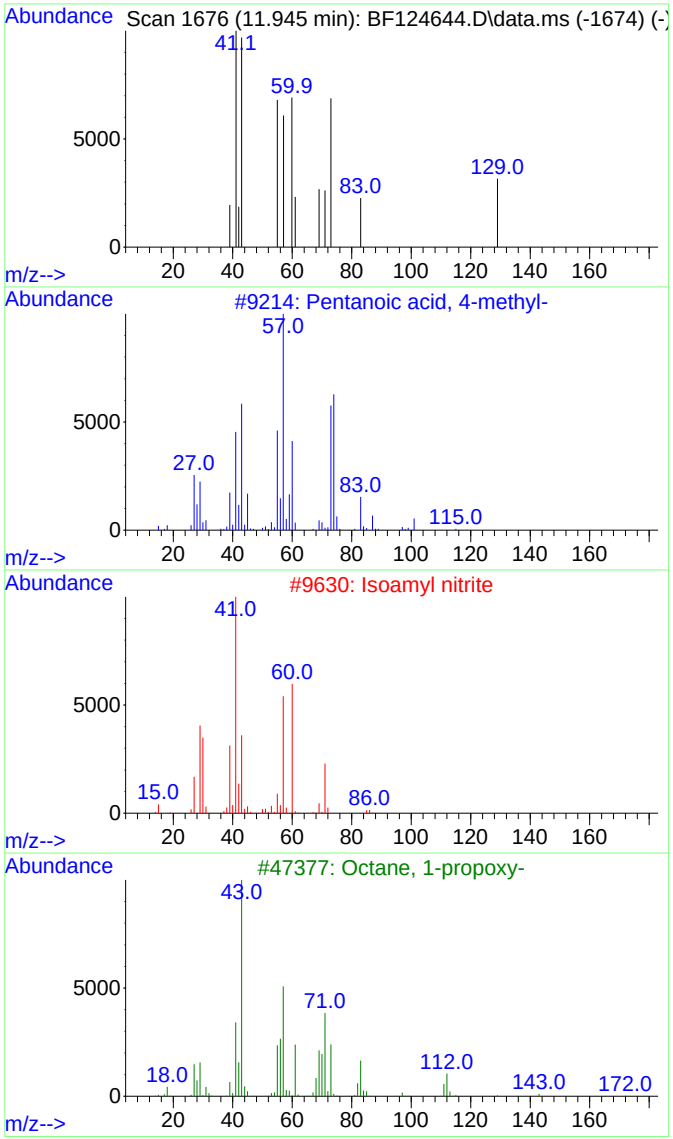
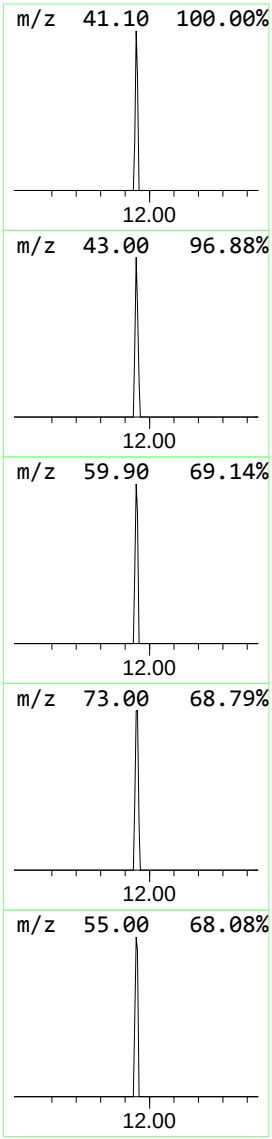
Peak Number 3 unknown11.945 Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.945 | 3.59 ng | 8079 | Phenanthrene-d10 | 11.427 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentanoic acid, 4-methyl- | 116 | C6H12O2 | 000646-07-1 | 25 |
| 2 | Isoamyl nitrite | 117 | C5H11NO2 | 000110-46-3 | 23 |
| 3 | Octane, 1-propoxy- | 172 | C11H24O | 029379-41-7 | 17 |
| 4 | 1-Hexanamine, 2-ethyl- | 129 | C8H19N | 000104-75-6 | 9 |
| 5 | 2,3,4,5-Tetrahydroxypentanal | 150 | C5H10O5 | 053106-52-8 | 9 |



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Operator : JU/CG
Sample : M3040-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-PS-01-076

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
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TIC Library : C:\Database\NIST20.L
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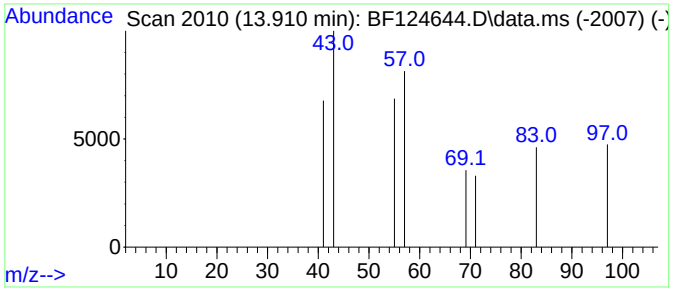
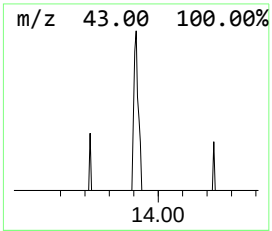
**********

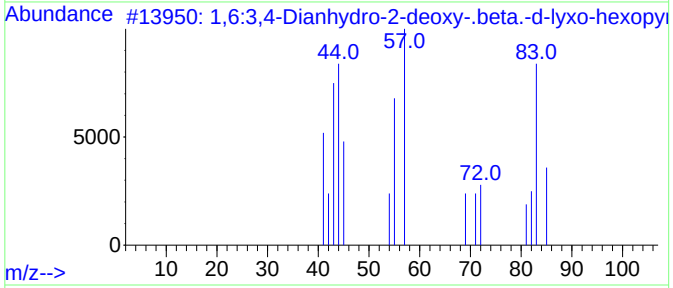
Peak Number 4 unknown13.910 Concentration Rank 4

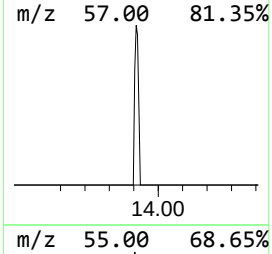
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.910 | 4.62 ng | 5373 | Chrysene-d12 | 14.068 |

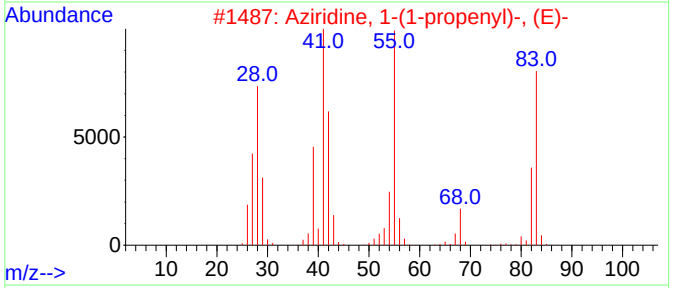
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,6:3,4-Dianhydro-2-deoxy-.beta.... | 128 | C6H8O3 | 050767-53-8 | 9 |
| 2 | Aziridine, 1-(1-propenyl)-, (E)- | 83 | C5H9N | 080839-91-4 | 7 |
| 3 | Pyridine, 2,3,4,5-tetrahydro- | 83 | C5H9N | 000505-18-0 | 4 |
| 4 | Octadecane, 2,2,4,15,17,17-hexam... | 591 | C42H86 | 055470-97-8 | 4 |
| 5 | 1-Allylazetidine | 97 | C6H11N | 1000195-02-5 | 4 |

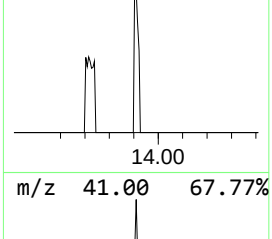


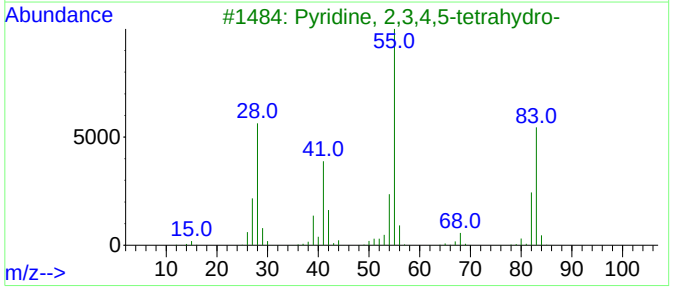



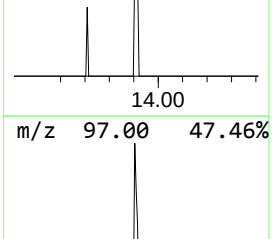



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

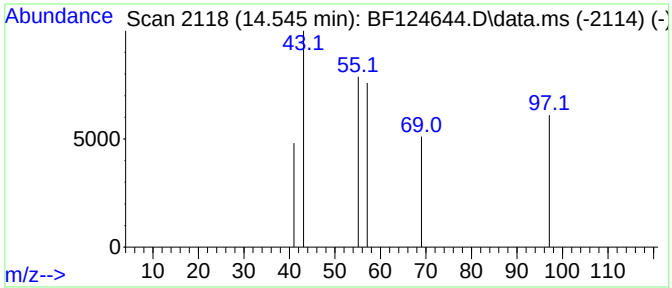
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

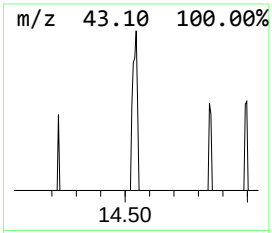
**********

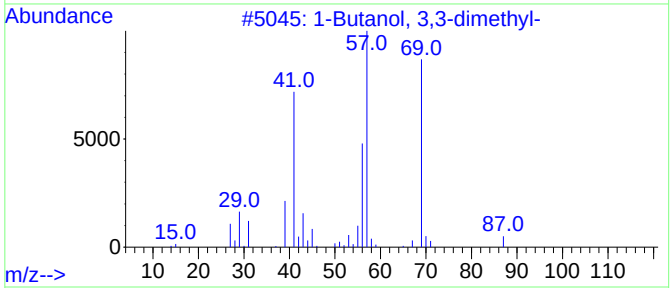
Peak Number 5 unknown14.545 Concentration Rank 7

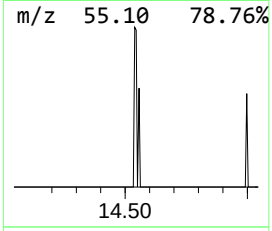
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.545 | 2.42 ng | 2819 | Chrysene-d12 | 14.068 |

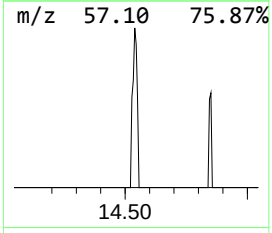
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Butanol, 3,3-dimethyl- | 102 | C6H14O | 000624-95-3 | 2 |
| 2 | 3,4-Hexanediol, 2,5-dimethyl- | 146 | C8H18O2 | 022607-11-0 | 2 |
| 3 | 1-Butyne, 3-ethoxy-3-methyl- | 112 | C7H12O | 007740-69-4 | 2 |
| 4 | 1H-Pyrrole-2,5-dione | 97 | C4H3NO2 | 000541-59-3 | 2 |
| 5 | 2,4,4-Trimethyl-1-pentanol, chlo... | 242 | C10H17ClF2O2 | 1000447-27-2 | 2 |

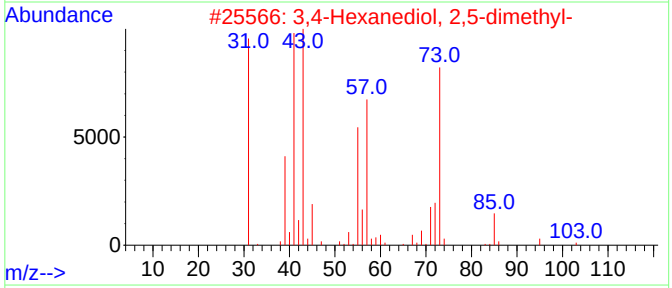


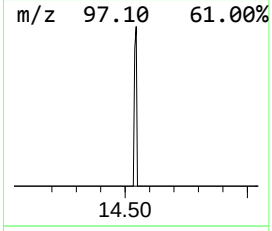



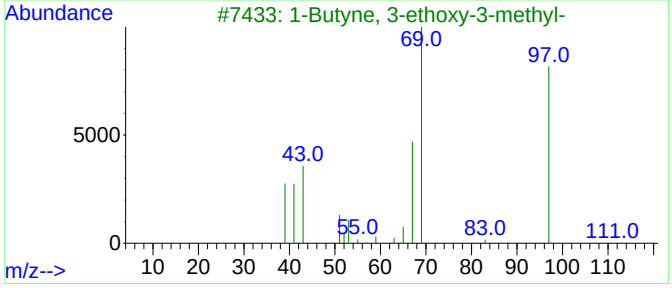



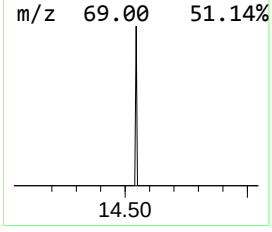



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

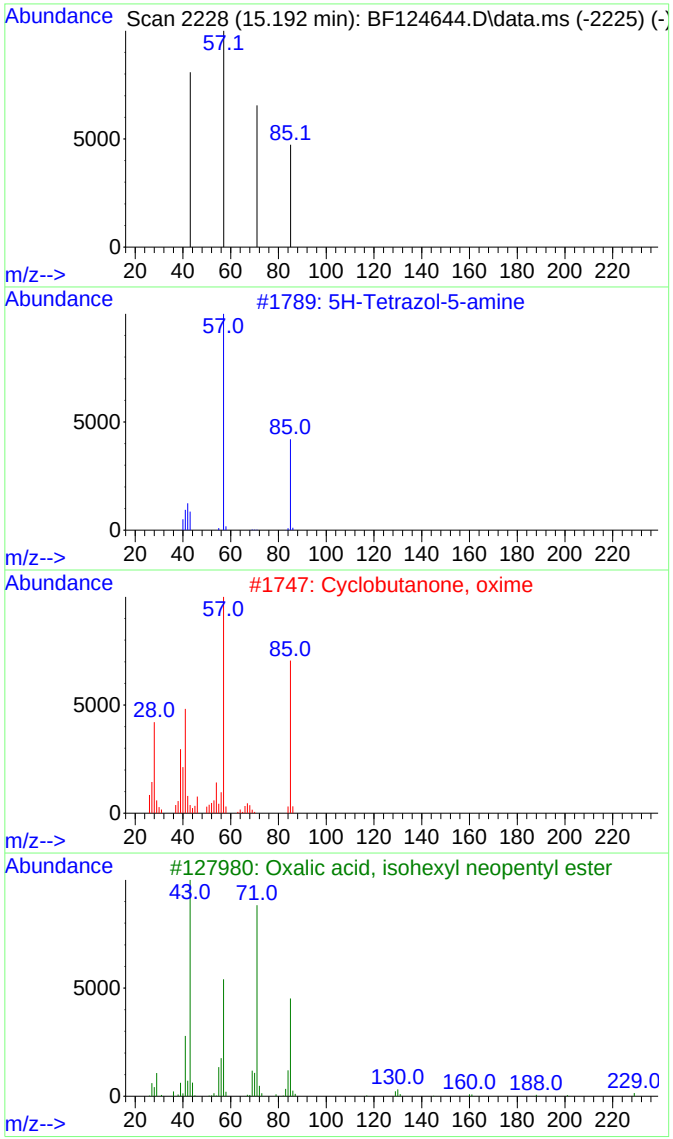
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

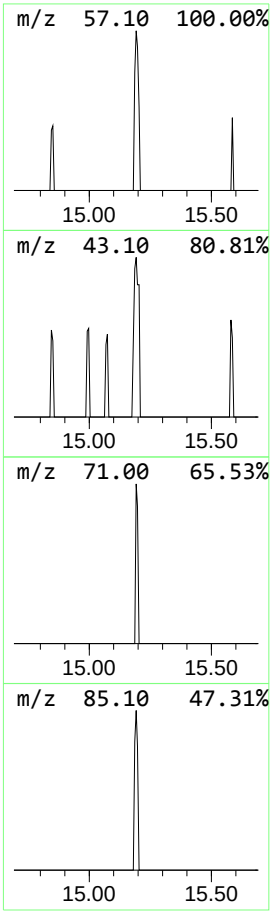
**********

Peak Number 6 unknown15.192 Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.192 | 2.50 ng | 2790 | Perylene-d12 | 15.557 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5H-Tetrazol-5-amine | 85 | CH3N5 | 1000273-02-0 | 4 |
| 2 | Cyclobutanone, oxime | 85 | C4H7NO | 002972-05-6 | 4 |
| 3 | Oxalic acid, isohexyl neopentyl ... | 244 | C13H24O4 | 1000309-73-0 | 4 |
| 4 | Azetidine, 2-methyl- | 71 | C4H9N | 019812-49-8 | 3 |
| 5 | Azetidine, 1-methyl- | 71 | C4H9N | 004923-79-9 | 3 |



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Data File : BF124644.D
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Sample : M3040-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
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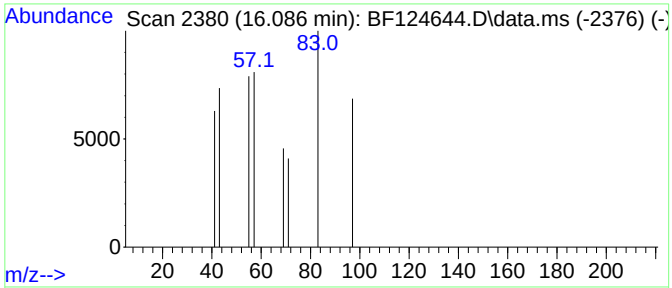
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

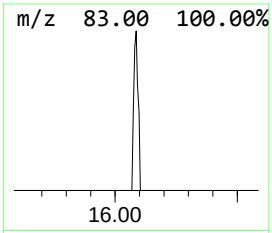
**********

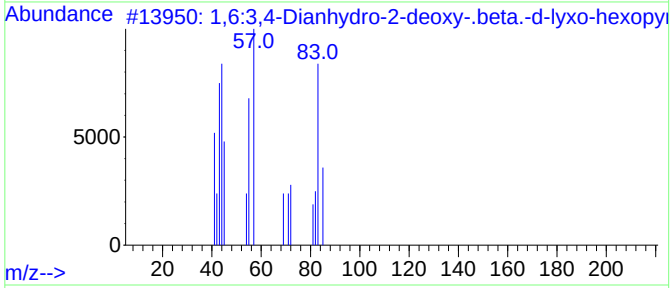
Peak Number 7 unknown16.086 Concentration Rank 2

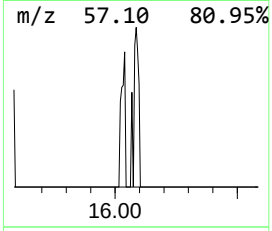
| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.086 | 4.99 ng | 5578 | Perylene-d12 | 15.557 |

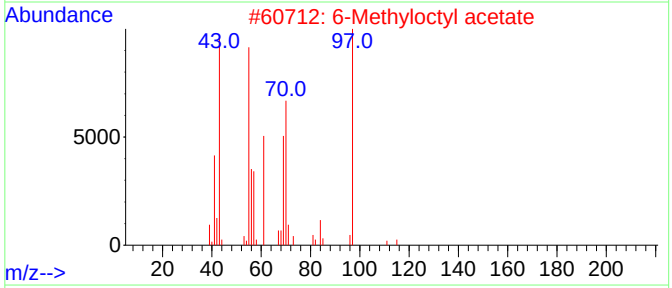
| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,6:3,4-Dianhydro-2-deoxy-.beta.... | 128 | C6H8O3 | 050767-53-8 | 36 |
| 2 | 6-Methyloctyl acetate | 186 | C11H22O2 | 1000439-66-5 | 9 |
| 3 | 2,4,4-Trimethyl-1-pentanol, trif... | 226 | C10H17F3O2 | 1000365-19-5 | 4 |
| 4 | 1-Allylazetidine | 97 | C6H11N | 1000195-02-5 | 4 |
| 5 | Azetidine, 2-methyl- | 71 | C4H9N | 019812-49-8 | 3 |

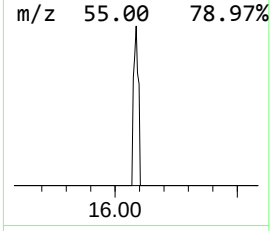


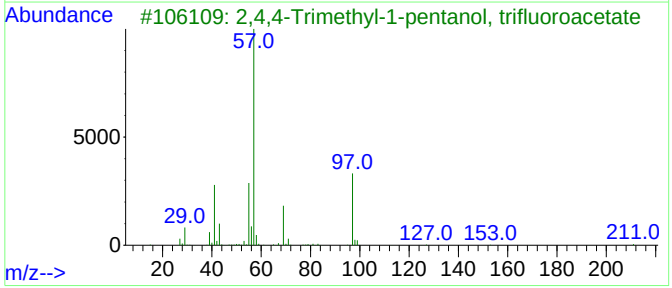



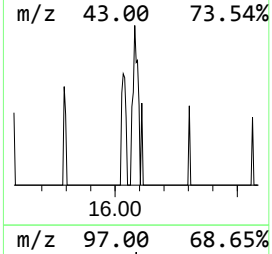



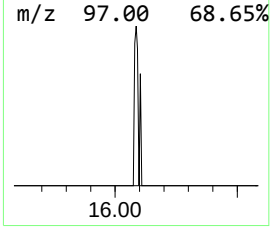



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072021\
Data File : BF124644.D
Acq On : 21 Jul 2021 00:20
Operator : JU/CG
Sample : M3040-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-PS-01-076

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| unknown2.222 | 2.222 | 4.8 | ng | 8706 | 1 | 6.904 | 35908 | 20.0 |
| Ethanol, 2-(2-b... | 8.081 | 5.2 | ng | 13252 | 2 | 8.186 | 50990 | 20.0 |
| unknown11.945 | 11.945 | 3.6 | ng | 8079 | 4 | 11.427 | 44976 | 20.0 |
| unknown13.910 | 13.910 | 4.6 | ng | 5373 | 5 | 14.068 | 23272 | 20.0 |
| unknown14.545 | 14.545 | 2.4 | ng | 2819 | 5 | 14.068 | 23272 | 20.0 |
| unknown15.192 | 15.192 | 2.5 | ng | 2790 | 6 | 15.557 | 22364 | 20.0 |
| unknown16.086 | 16.086 | 5.0 | ng | 5578 | 6 | 15.557 | 22364 | 20.0 |