LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030422\
Data File : BF127208.D
Acq On : 04 Mar 2022 18:42
Operator : CG\JU
Sample : N1793-10
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
SB-4

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-BF021622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127208.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 5.498 | 542 | 546 | 558 | rBV | 1052980 | 981841 | 29.68% | 5.308% |
| 2 | 5.898 | 610 | 614 | 626 | rVB | 71854 | 65119 | 1.97% | 0.352% |
| 3 | 6.504 | 713 | 717 | 733 | rVB | 505830 | 582392 | 17.60% | 3.149% |
| 4 | 6.875 | 776 | 780 | 784 | rBV | 656730 | 532426 | 16.09% | 2.878% |
| 5 | 7.022 | 802 | 805 | 814 | rBV | 418384 | 341132 | 10.31% | 1.844% |
| 6 | 7.445 | 871 | 877 | 880 | rBV | 1814827 | 1823933 | 55.13% | 9.861% |
| 7 | 7.539 | 886 | 893 | 900 | rBV | 101766 | 149589 | 4.52% | 0.809% |
| 8 | 8.157 | 994 | 998 | 1002 | rBV | 773290 | 698144 | 21.10% | 3.774% |
| 9 | 9.239 | 1176 | 1182 | 1185 | rBV | 3516960 | 3308189 | 100.00% | 17.885% |
| 10 | 9.916 | 1291 | 1297 | 1301 | rVB | 943214 | 843955 | 25.51% | 4.563% |
| 11 | 10.716 | 1427 | 1433 | 1436 | rBV | 2519812 | 2368057 | 71.58% | 12.802% |
| 12 | 11.410 | 1547 | 1551 | 1554 | rBV | 1123885 | 894402 | 27.04% | 4.835% |
| 13 | 11.792 | 1612 | 1616 | 1619 | rBV | 863336 | 676370 | 20.45% | 3.657% |
| 14 | 11.822 | 1619 | 1621 | 1624 | rVB | 48941 | 40318 | 1.22% | 0.218% |
| 15 | 12.998 | 1817 | 1821 | 1824 | rBV | 3396372 | 3255976 | 98.42% | 17.602% |
| 16 | 13.921 | 1974 | 1978 | 1981 | rVB | 40566 | 40117 | 1.21% | 0.217% |
| 17 | 14.057 | 1997 | 2001 | 2007 | rVB | 833202 | 721972 | 21.82% | 3.903% |
| 18 | 14.151 | 2011 | 2017 | 2023 | rBV | 335120 | 366580 | 11.08% | 1.982% |
| 19 | 14.821 | 2126 | 2131 | 2134 | rBV2 | 31023 | 36046 | 1.09% | 0.195% |
| 20 | 15.163 | 2185 | 2189 | 2194 | rVB | 36694 | 41929 | 1.27% | 0.227% |
| 21 | 15.545 | 2246 | 2254 | 2263 | rBV | 470443 | 579613 | 17.52% | 3.134% |
| 22 | 15.998 | 2325 | 2331 | 2340 | rVB2 | 31248 | 52548 | 1.59% | 0.284% |
| 23 | 16.509 | 2413 | 2418 | 2427 | rVB4 | 28771 | 51404 | 1.55% | 0.278% |
| 24 | 17.121 | 2517 | 2522 | 2529 | rVB3 | 21504 | 45214 | 1.37% | 0.244% |

Sum of corrected areas: 18497266

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**ClientSampleId :**
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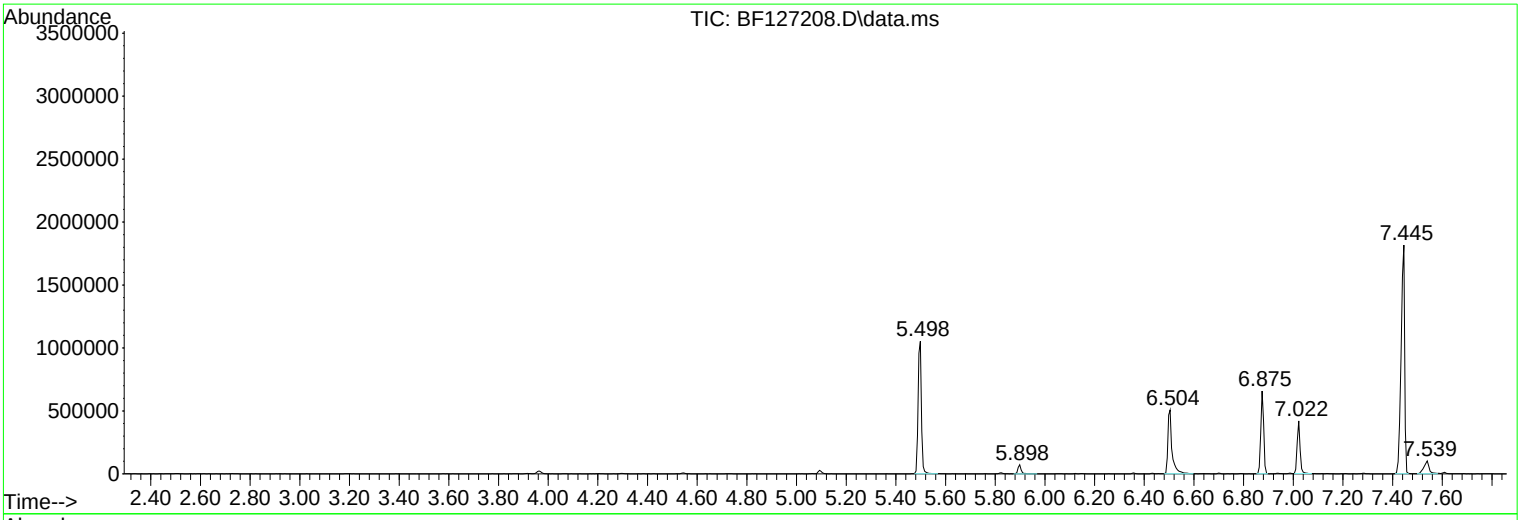
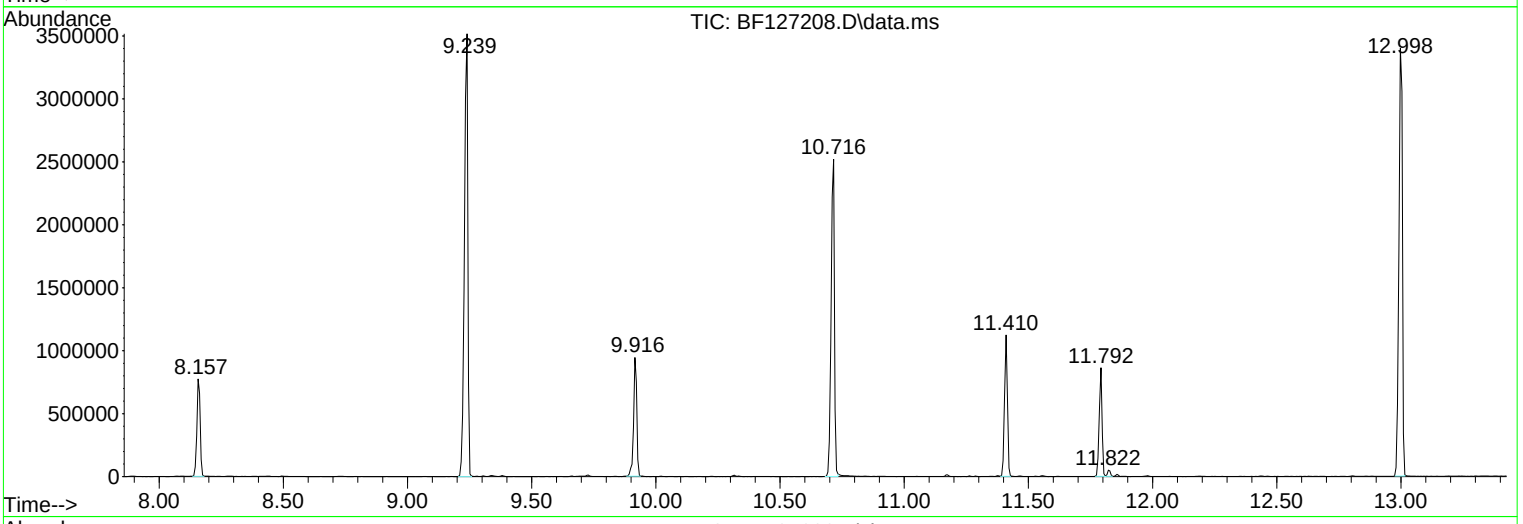
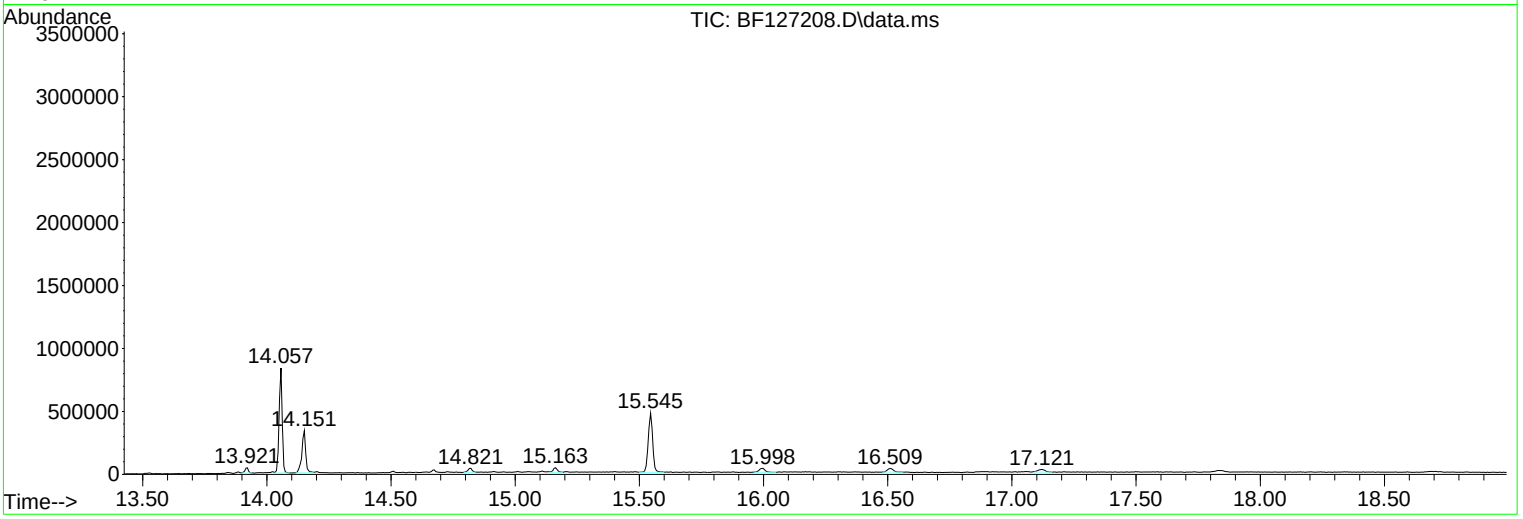
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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**Instrument :**
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

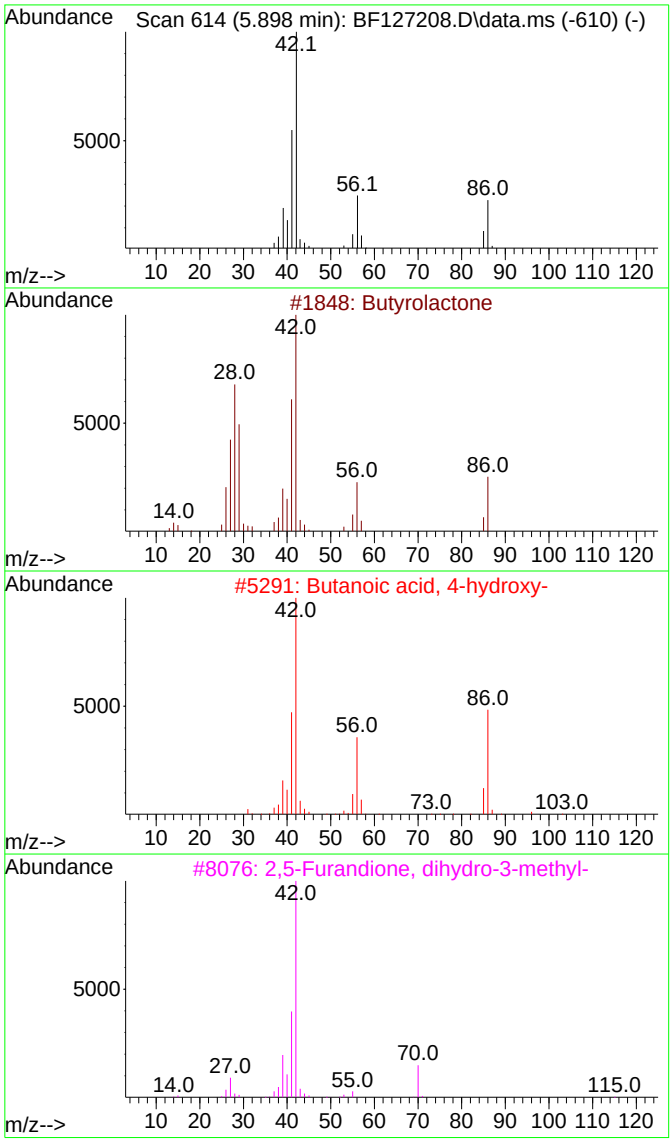
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

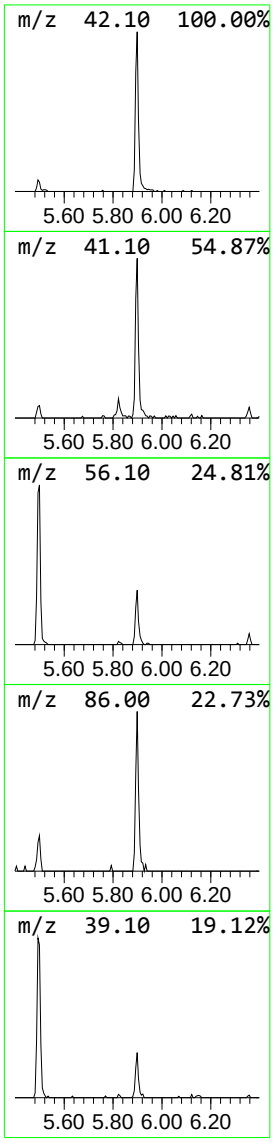
**********

Peak Number 1 Butyrolactone Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.898 | 2.45 ng | 65119 | 1,4-Dichlorobenzene-d4 | 6.875 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Butyrolactone | 86 | C4H6O2 | 000096-48-0 | 86 |
| 2 | Butanoic acid, 4-hydroxy- | 104 | C4H8O3 | 000591-81-1 | 83 |
| 3 | 2,5-Furandione, dihydro-3-methyl- | 114 | C5H6O3 | 004100-80-5 | 50 |
| 4 | 1-Propanamine, N,2-dimethyl-N-ni... | 116 | C5H12N2O | 034419-76-6 | 36 |
| 5 | Azetidine, 1-nitroso- | 86 | C3H6N2O | 015216-10-1 | 12 |



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Sample : N1793-10
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
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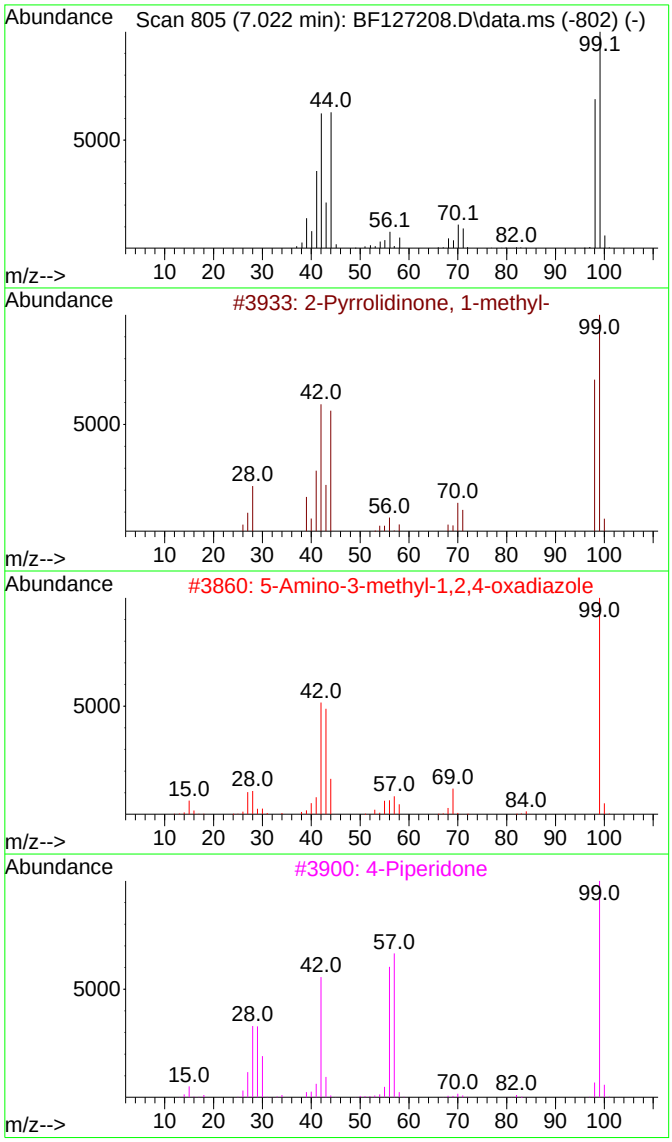
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

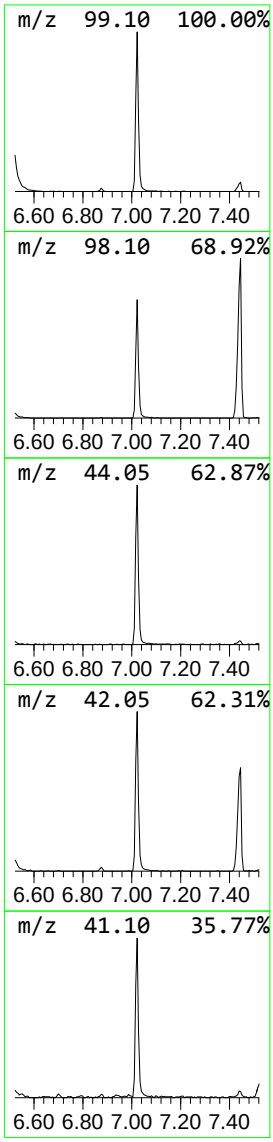
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 2 2-Pyrrolidinone, 1-methyl- Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.022 | 12.81 ng | 341132 | 1,4-Dichlorobenzene-d4 | 6.875 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pyrrolidinone, 1-methyl- | 99 | C5H9NO | 000872-50-4 | 95 |
| 2 | 5-Amino-3-methyl-1,2,4-oxadiazole | 99 | C3H5N3O | 003663-39-6 | 43 |
| 3 | 4-Piperidone | 99 | C5H9NO | 041661-47-6 | 37 |
| 4 | 2-Piperidinone | 99 | C5H9NO | 000675-20-7 | 37 |
| 5 | Allyl Isothiocyanate | 99 | C4H5NS | 000057-06-7 | 32 |



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Operator : CG\JU
Sample : N1793-10
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

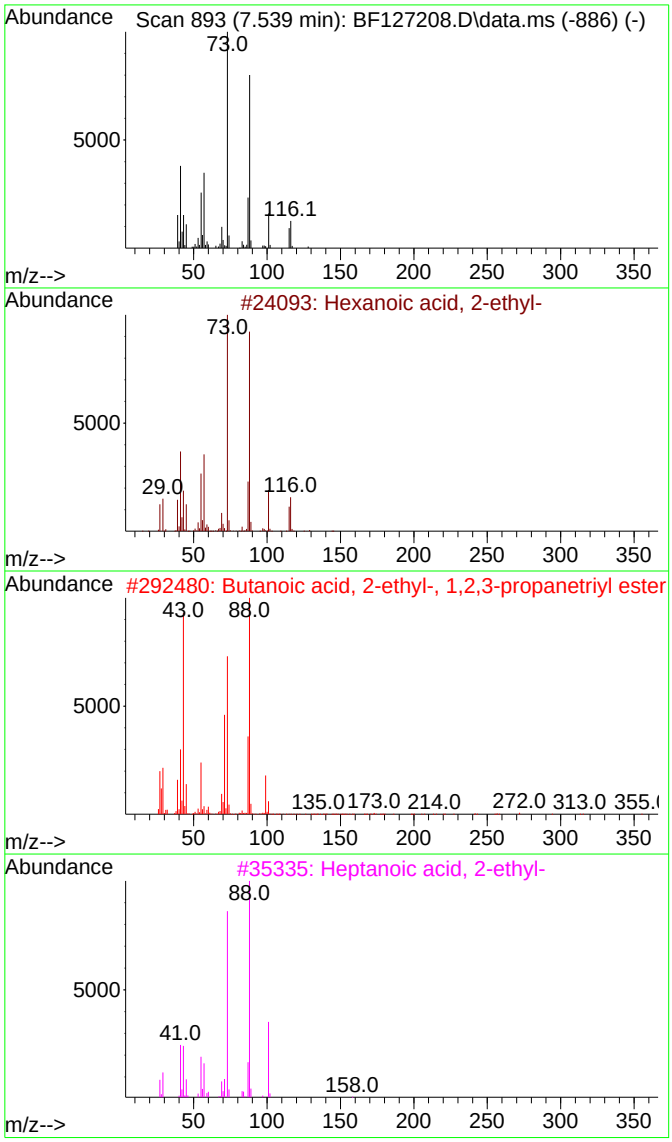
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

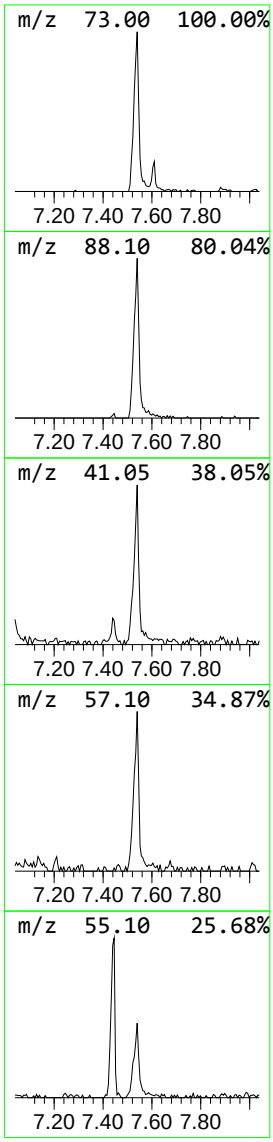
**********

Peak Number 3 Hexanoic acid, 2-ethyl- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.539 | 4.29 ng | 149589 | Naphthalene-d8 | 8.157 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexanoic acid, 2-ethyl- | 144 | C8H16O2 | 000149-57-5 | 91 |
| 2 | Butanoic acid, 2-ethyl-, 1,2,3-p... | 386 | C21H38O6 | 056554-54-2 | 59 |
| 3 | Heptanoic acid, 2-ethyl- | 158 | C9H18O2 | 003274-29-1 | 53 |
| 4 | Acetic acid, diethyl- | 116 | C6H12O2 | 000088-09-5 | 45 |
| 5 | 2-Ethyl-4-methylpentanoic acid | 144 | C8H16O2 | 000108-81-6 | 45 |



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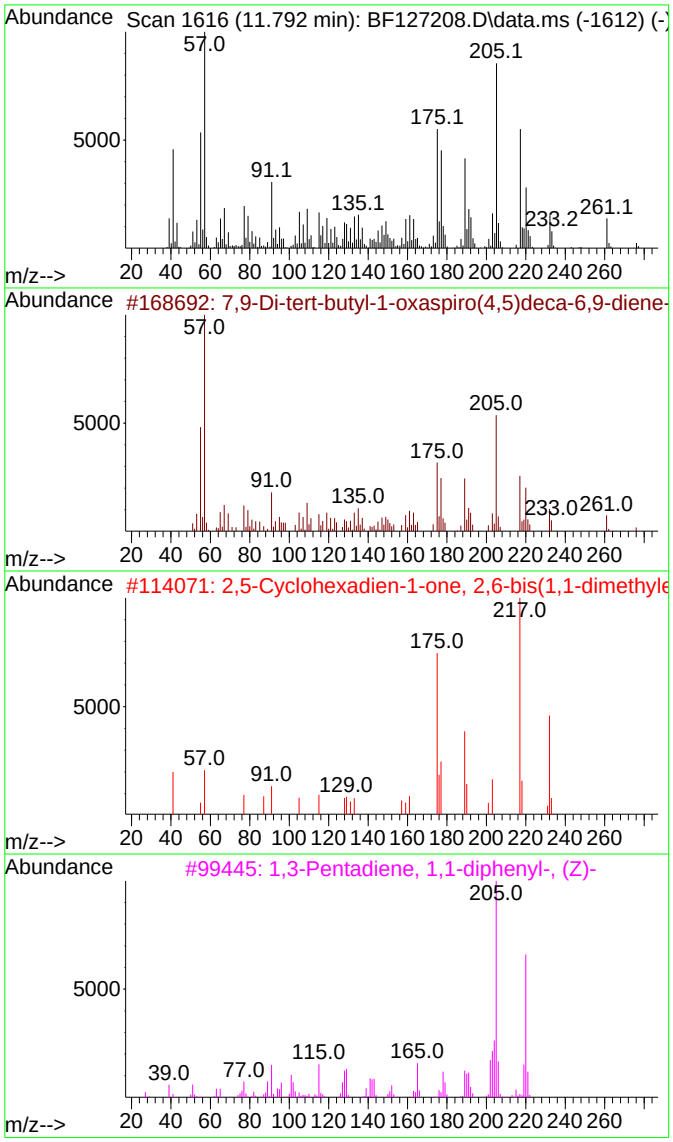
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

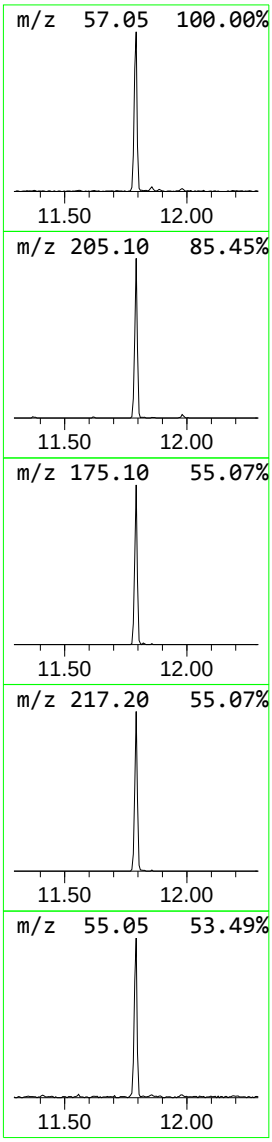
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 4 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.792 | 15.12 ng | 676370 | Phenanthrene-d10 | 11.410 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 7,9-Di-tert-butyl-1-oxaspiro(4,5... | 276 | C17H24O3 | 082304-66-3 | 99 |
| 2 | 2,5-Cyclohexadien-1-one, 2,6-bis... | 232 | C16H24O | 006738-27-8 | 80 |
| 3 | 1,3-Pentadiene, 1,1-diphenyl-, (Z)- | 220 | C17H16 | 015295-31-5 | 51 |
| 4 | Ethanone, 1-(5,6,7,8-tetrahydro-... | 220 | C14H20O2 | 071596-88-8 | 50 |
| 5 | (Z)-((2-Benzylideneheptyl)oxy)tr... | 276 | C17H28OSi | 1000495-65-9 | 48 |



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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
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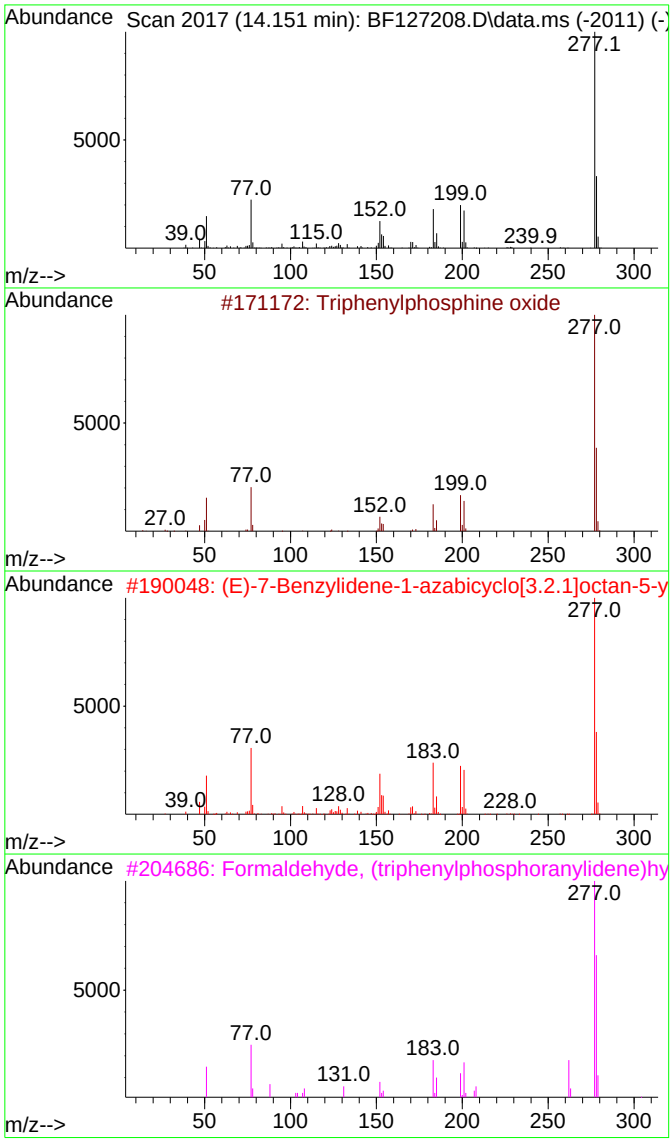
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

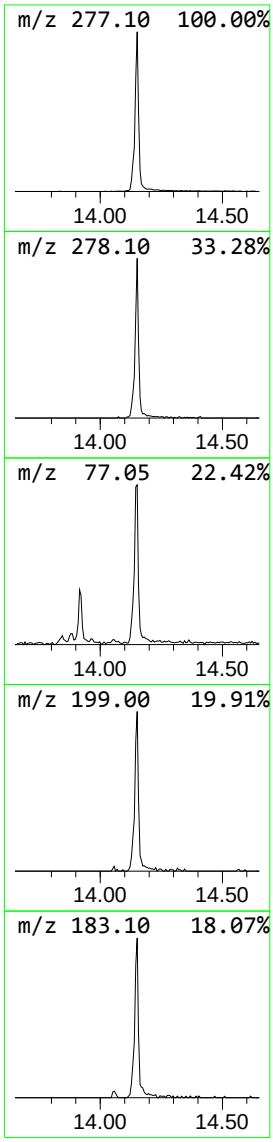
**********

Peak Number 5 Triphenylphosphine oxide Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.151 | 10.15 ng | 366580 | Chrysene-d12 | 14.057 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Triphenylphosphine oxide | 278 | C18H15OP | 000791-28-6 | 93 |
| 2 | (E)-7-Benzylidene-1-azabicyclo[3... | 293 | C15H19NO3S | 1000483-83-4 | 91 |
| 3 | Formaldehyde, (triphenylphosphor... | 304 | C19H17N2P | 015990-54-2 | 45 |
| 4 | Vanadium, cycloheptatrienyl-(pen... | 277 | C17H22V | 1000155-20-5 | 28 |
| 5 | Cobalt,(.eta.<5>-2,4-cyclopentad... | 277 | C16H15BCo | 036682-12-9 | 23 |



Tentatively Identified Compound (LSC) summary

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

| | | | | | --Internal Standard--- | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| Butyrolactone | 5.898 | 2.5 | ng | 65119 | 1 | 6.875 | 532426 | 20.0 |
| 2-Pyrrolidinone... | 7.022 | 12.8 | ng | 341132 | 1 | 6.875 | 532426 | 20.0 |
| Hexanoic acid, ... | 7.539 | 4.3 | ng | 149589 | 2 | 8.157 | 698144 | 20.0 |
| 7,9-Di-tert-but... | 11.792 | 15.1 | ng | 676370 | 4 | 11.410 | 894402 | 20.0 |
| Triphenylphosph... | 14.151 | 10.2 | ng | 366580 | 5 | 14.057 | 721972 | 20.0 |