LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120622\
Data File : BF131536.D
Acq On : 06 Dec 2022 20:00
Operator : CG\JU
Sample : N5870-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
ML-2

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-BF120522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131536.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.246 | 19 | 27 | 33 | rVB | 463011 | 605212 | 14.40% | 2.547% |
| 2 | 2.358 | 41 | 46 | 52 | rVB | 41341 | 49832 | 1.19% | 0.210% |
| 3 | 5.151 | 515 | 521 | 532 | rVB | 551410 | 833234 | 19.83% | 3.506% |
| 4 | 5.546 | 582 | 588 | 591 | rBV | 2515060 | 2592482 | 61.68% | 10.910% |
| 5 | 5.934 | 650 | 654 | 657 | rBV | 79275 | 63350 | 1.51% | 0.267% |
| 6 | 6.551 | 752 | 759 | 761 | rBV | 2124473 | 2627536 | 62.52% | 11.057% |
| 7 | 6.922 | 818 | 822 | 825 | rBV | 610277 | 496046 | 11.80% | 2.087% |
| 8 | 7.492 | 912 | 919 | 922 | rBV | 1650610 | 1725601 | 41.06% | 7.262% |
| 9 | 7.745 | 958 | 962 | 966 | rBV | 175879 | 155036 | 3.69% | 0.652% |
| 10 | 8.210 | 1036 | 1041 | 1044 | rBV | 737882 | 628059 | 14.94% | 2.643% |
| 11 | 9.292 | 1219 | 1225 | 1228 | rBV | 4556894 | 4004396 | 95.28% | 16.851% |
| 12 | 9.975 | 1335 | 1341 | 1344 | rBV | 951406 | 786309 | 18.71% | 3.309% |
| 13 | 10.692 | 1459 | 1463 | 1466 | rBV | 162609 | 124981 | 2.97% | 0.526% |
| 14 | 10.769 | 1471 | 1476 | 1479 | rBV | 3283944 | 2828099 | 67.29% | 11.901% |
| 15 | 10.875 | 1489 | 1494 | 1500 | rVB | 100411 | 96373 | 2.29% | 0.406% |
| 16 | 11.469 | 1591 | 1595 | 1598 | rBV | 1067771 | 847817 | 20.17% | 3.568% |
| 17 | 13.069 | 1861 | 1867 | 1870 | rBV | 4507227 | 4202778 | 100.00% | 17.686% |
| 18 | 14.039 | 2023 | 2032 | 2042 | rBV10 | 23676 | 112820 | 2.68% | 0.475% |
| 19 | 14.121 | 2042 | 2046 | 2053 | rVB | 631069 | 550433 | 13.10% | 2.316% |
| 20 | 15.639 | 2298 | 2304 | 2317 | rVB | 340245 | 432793 | 10.30% | 1.821% |

Sum of corrected areas: 23763187

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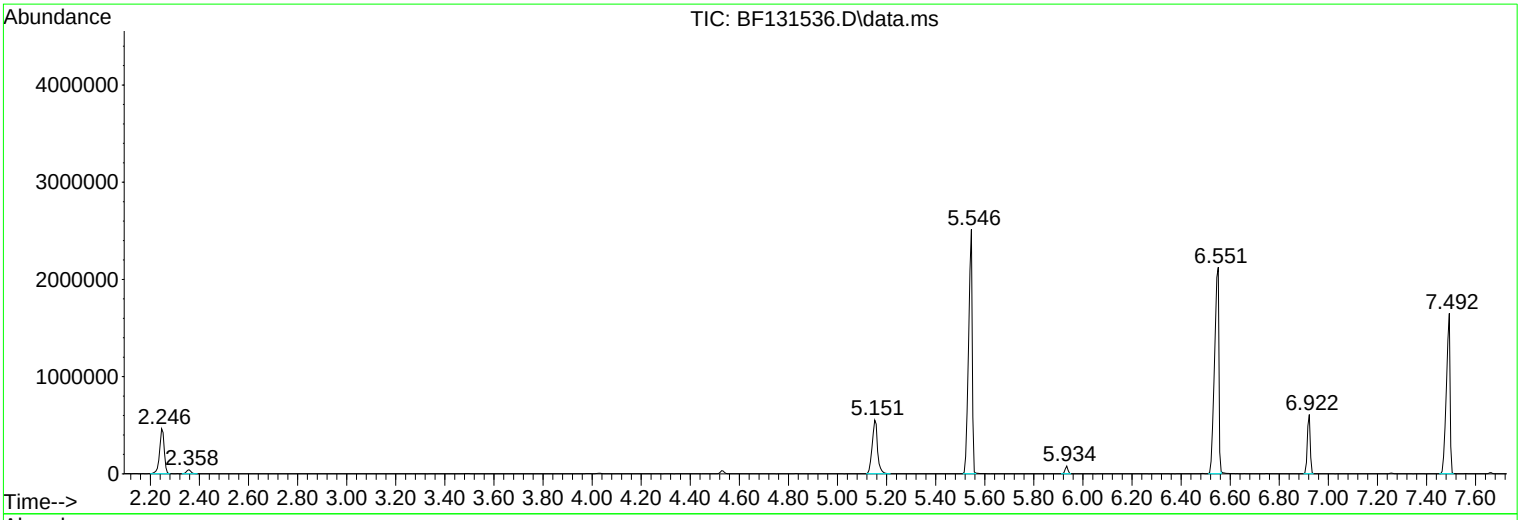
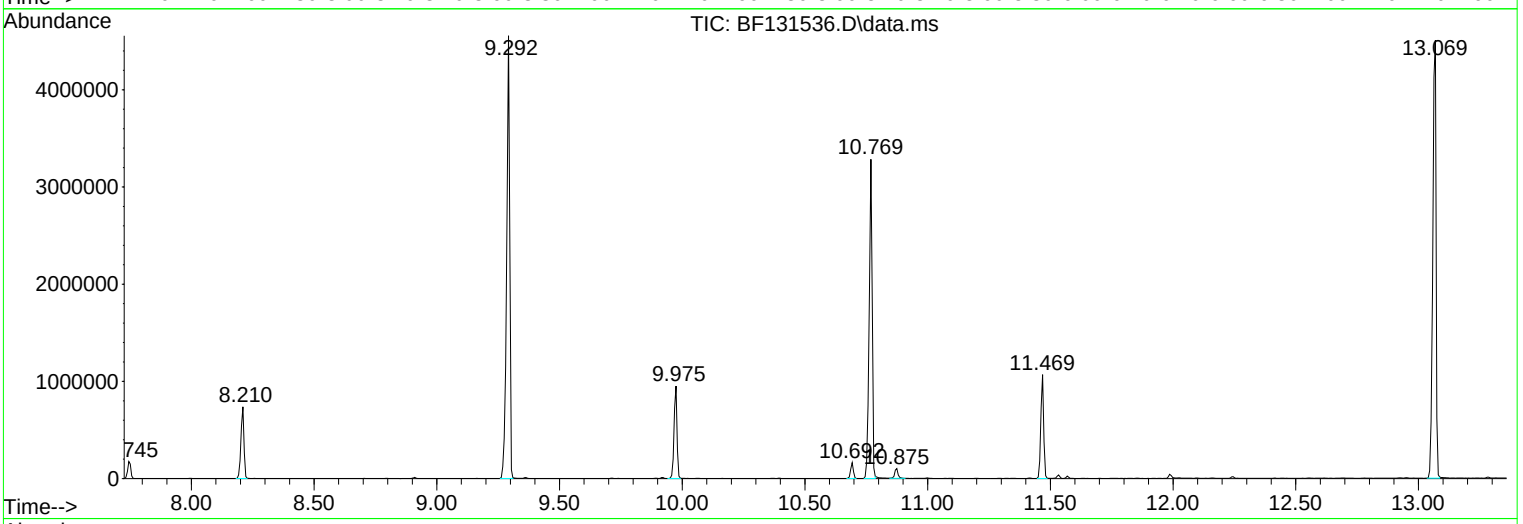
Misc :
ALS Vial : 19 Sample Multiplier: 1

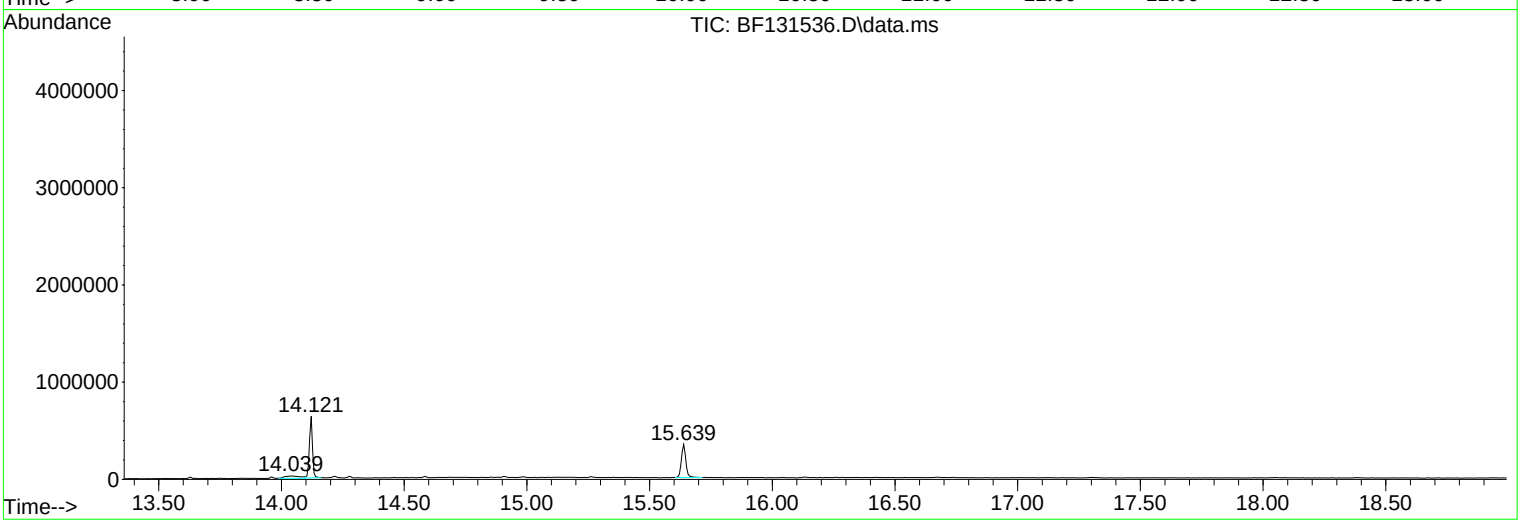
**Instrument :**
BNA_F
**ClientSampleId :**
ML-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120522.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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Data File : BF131536.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

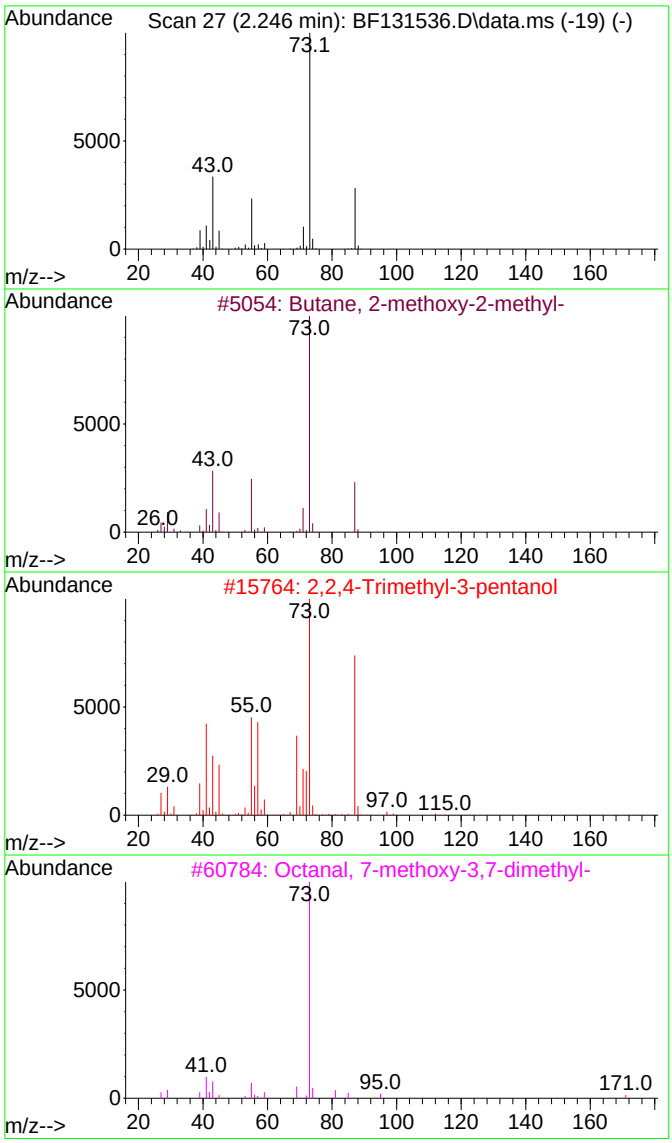
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

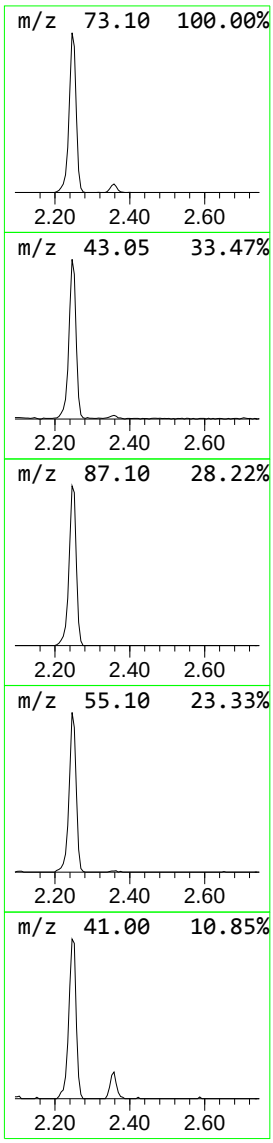
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.246 | 24.40 ng | 605212 | 1,4-Dichlorobenzene-d4 | 6.922 |

| 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 | Octanal, 7-methoxy-3,7-dimethyl- | 186 | C11H22O2 | 003613-30-7 | 25 |
| 4 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 23 |
| 5 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 9 |



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Data File : BF131536.D
Acq On : 06 Dec 2022 20:00
Operator : CG\JU
Sample : N5870-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
ML-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

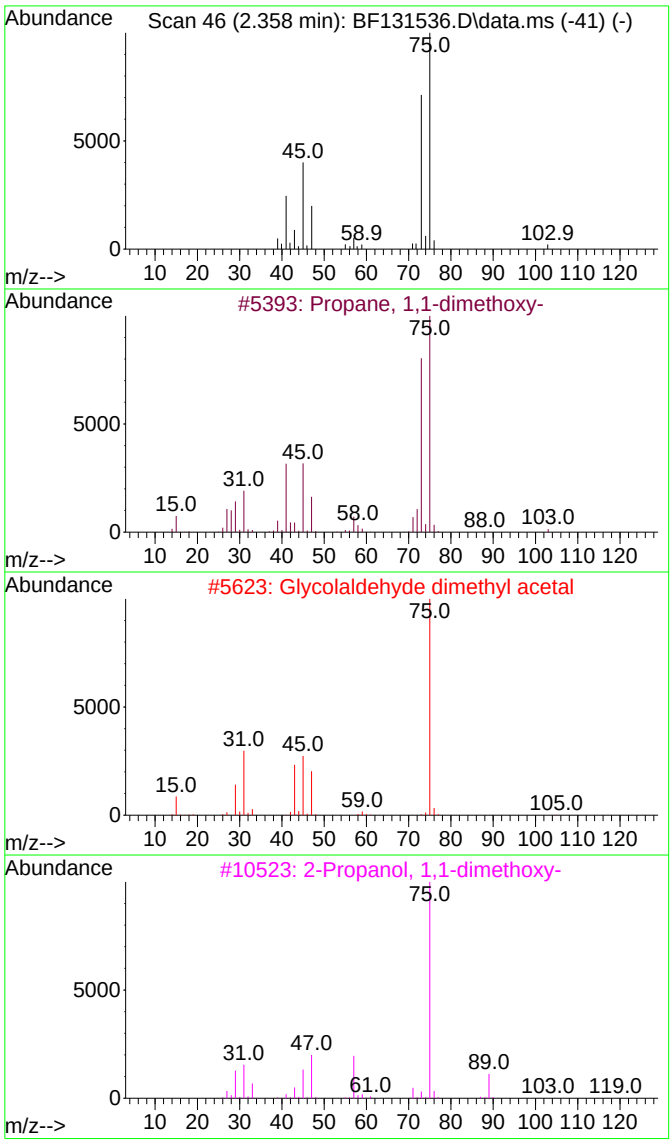
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

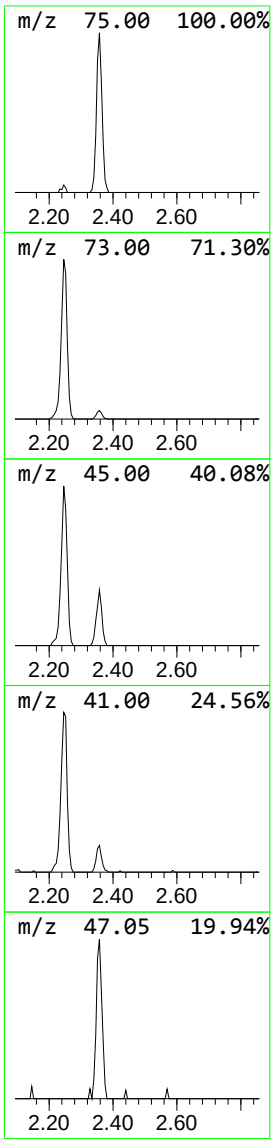
**********

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.358 | 2.01 ng | 49832 | 1,4-Dichlorobenzene-d4 | 6.922 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propane, 1,1-dimethoxy- | 104 | C5H12O2 | 004744-10-9 | 83 |
| 2 | Glycolaldehyde dimethyl acetal | 106 | C4H10O3 | 030934-97-5 | 56 |
| 3 | 2-Propanol, 1,1-dimethoxy- | 120 | C5H12O3 | 042919-42-6 | 36 |
| 4 | 2,5-Diethoxy-3-methyl-3-vinylhexane | 214 | C13H26O2 | 1000432-70-8 | 22 |
| 5 | Pentane, 3-methoxy- | 102 | C6H14O | 036839-67-5 | 14 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120622\
Data File : BF131536.D
Acq On : 06 Dec 2022 20:00
Operator : CG\JU
Sample : N5870-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
ML-2

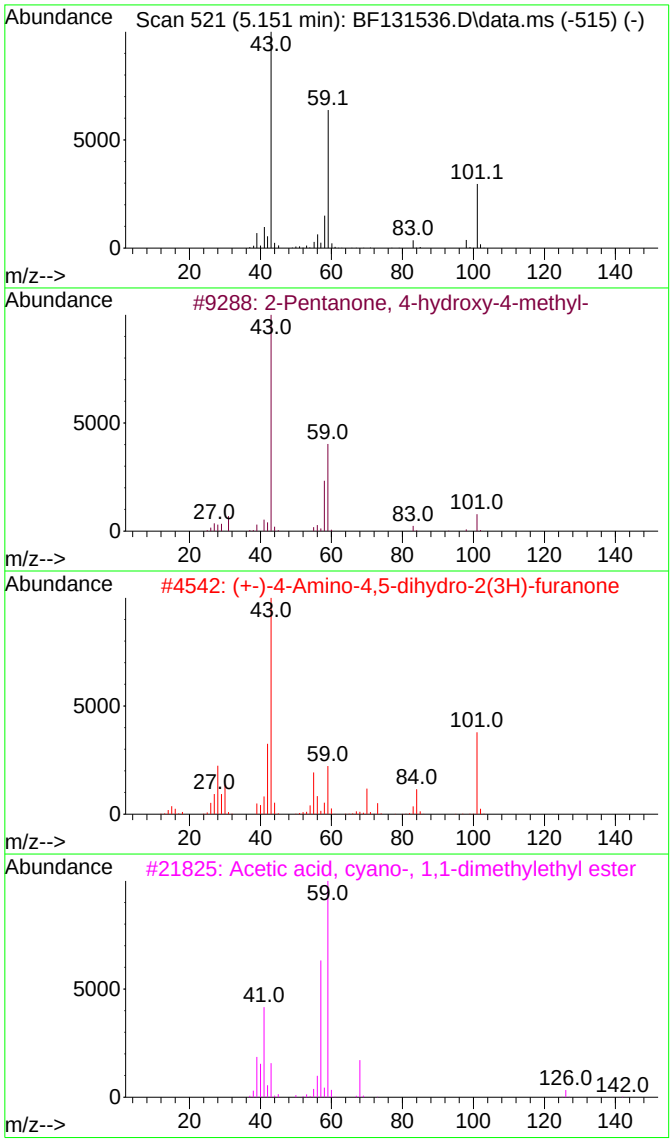
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

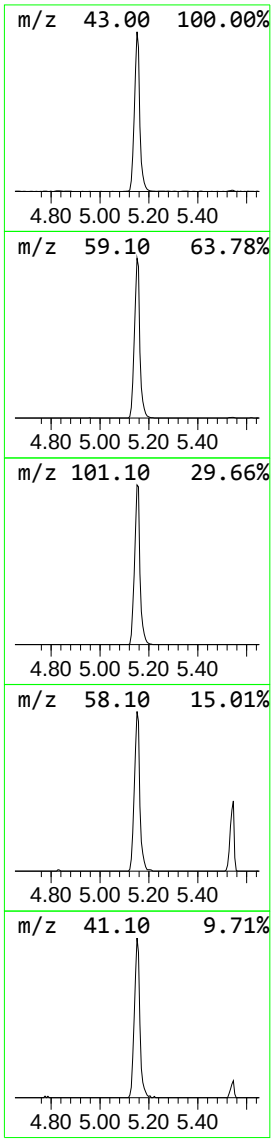
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.151 | 33.59 ng | 833234 | 1,4-Dichlorobenzene-d4 | 6.922 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 59 |
| 2 | (+-)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 47 |
| 3 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25 |
| 4 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 10 |
| 5 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |



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Acq On : 06 Dec 2022 20:00
Operator : CG\JU
Sample : N5870-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
ML-2

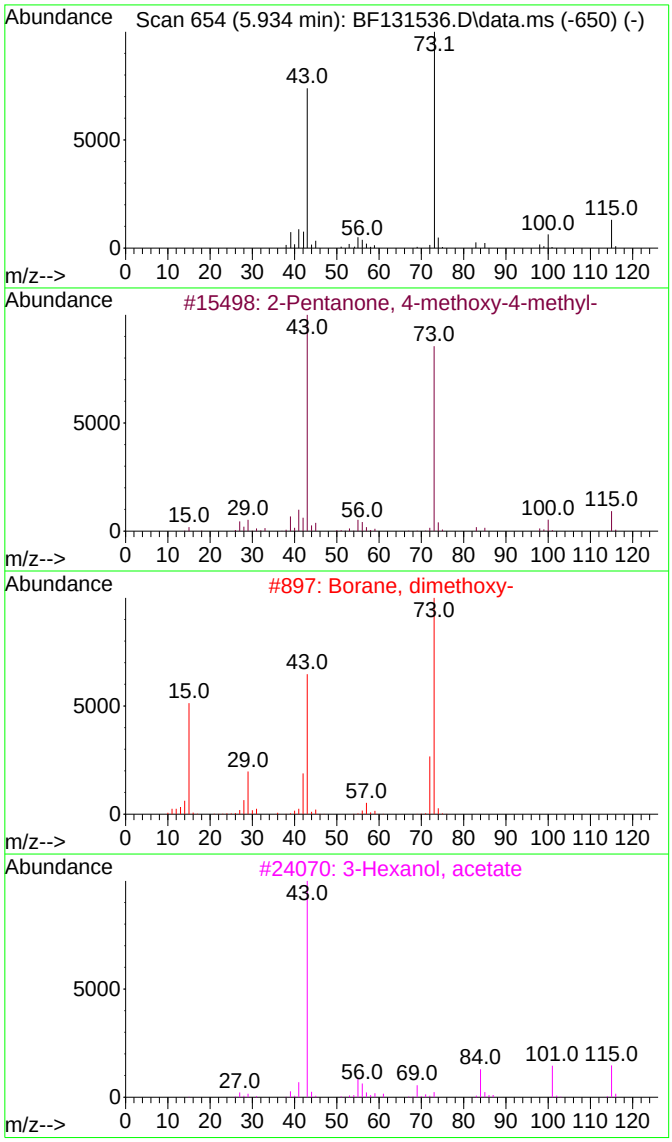
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

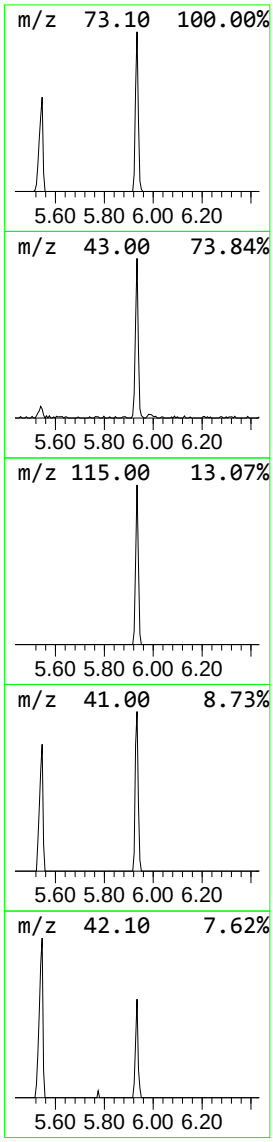
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.934 | 2.55 ng | 63350 | 1,4-Dichlorobenzene-d4 | 6.922 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-methoxy-4-methyl- | 130 | C7H14O2 | 000107-70-0 | 72 |
| 2 | Borane, dimethoxy- | 74 | C2H7BO2 | 004542-61-4 | 40 |
| 3 | 3-Hexanol, acetate | 144 | C8H16O2 | 040780-64-1 | 37 |
| 4 | N-.alpha.-Acetylglycinamide | 116 | C4H8N2O2 | 002620-63-5 | 33 |
| 5 | Butane, 2-methoxy-2,3,3-trimethyl- | 130 | C8H18O | 027705-21-1 | 25 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120622\
Data File : BF131536.D
Acq On : 06 Dec 2022 20:00
Operator : CG\JU
Sample : N5870-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
ML-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

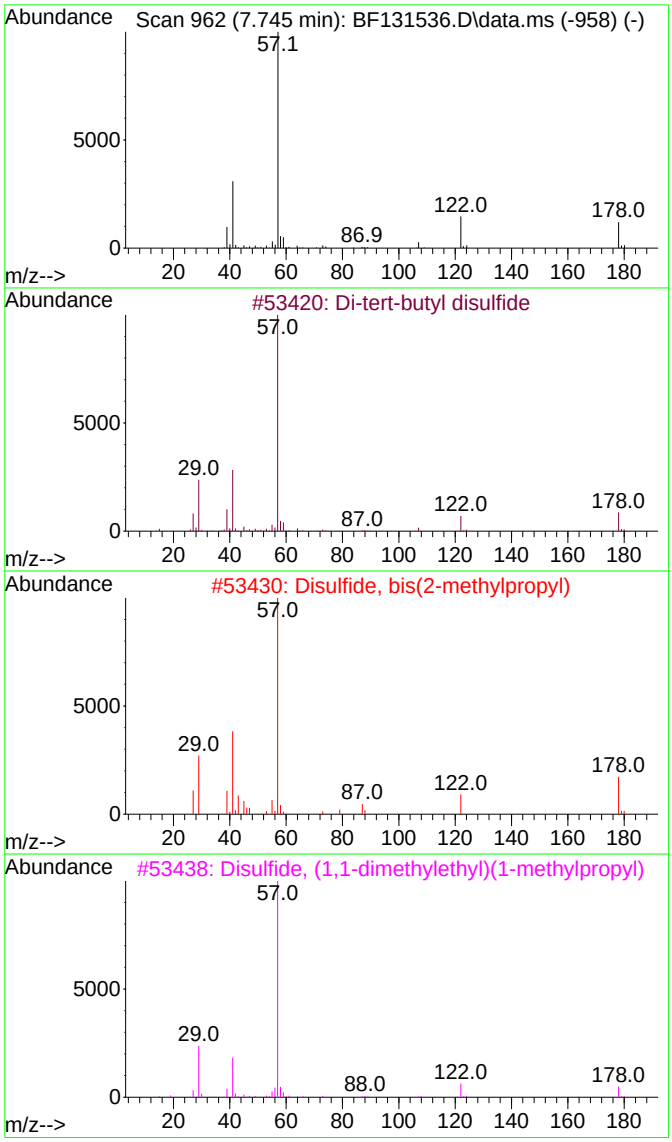
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

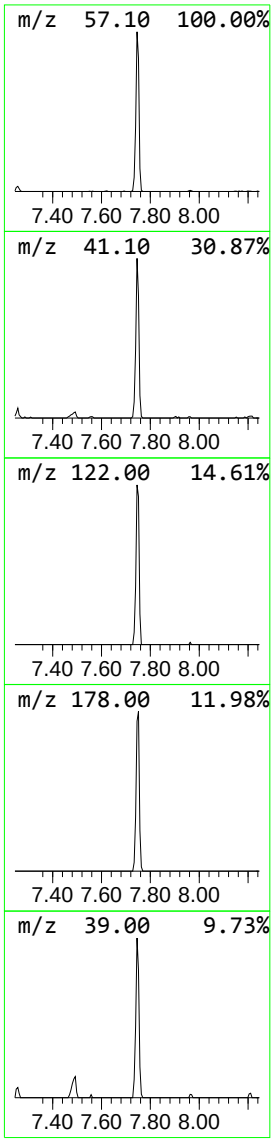
**********

Peak Number 5 Di-tert-butyl disulfide Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.745 | 4.94 ng | 155036 | Naphthalene-d8 | 8.210 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Di-tert-butyl disulfide | 178 | C8H18S2 | 000110-06-5 | 81 |
| 2 | Disulfide, bis(2-methylpropyl) | 178 | C8H18S2 | 001518-72-5 | 64 |
| 3 | Disulfide, (1,1-dimethylethyl)(1... | 178 | C8H18S2 | 072437-46-8 | 64 |
| 4 | Disulfide, bis(1-methylpropyl) | 178 | C8H18S2 | 005943-30-6 | 64 |
| 5 | Disulfide, (1-methylethyl) (1,1-... | 164 | C7H16S2 | 043022-60-2 | 43 |



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Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

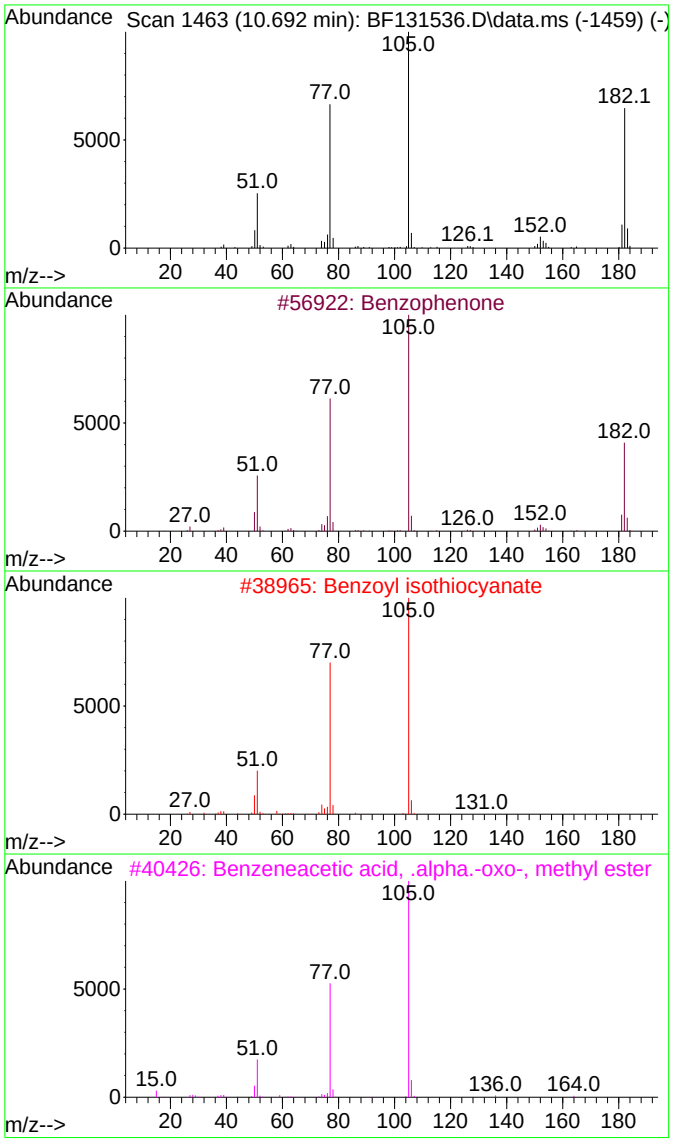
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

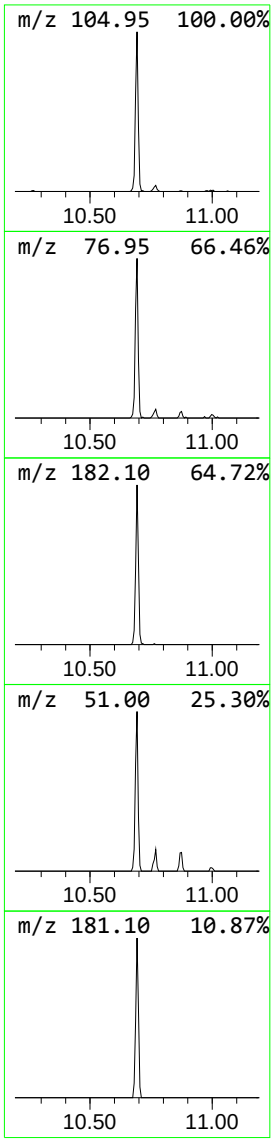
**********

Peak Number 6 Benzophenone Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.692 | 3.18 ng | 124981 | Acenaphthene-d10 | 9.975 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzophenone | 182 | C13H10O | 000119-61-9 | 96 |
| 2 | Benzoyl isothiocyanate | 163 | C8H5NOS | 000532-55-8 | 43 |
| 3 | Benzeneacetic acid, .alpha.-oxo-... | 164 | C9H8O3 | 015206-55-0 | 43 |
| 4 | 1-Propanone, 2-bromo-1-phenyl- | 212 | C9H9BrO | 002114-00-3 | 43 |
| 5 | Benzenecarbothioic acid, S-methy... | 152 | C8H8OS | 005925-68-8 | 43 |



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Sample : N5870-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
ML-2

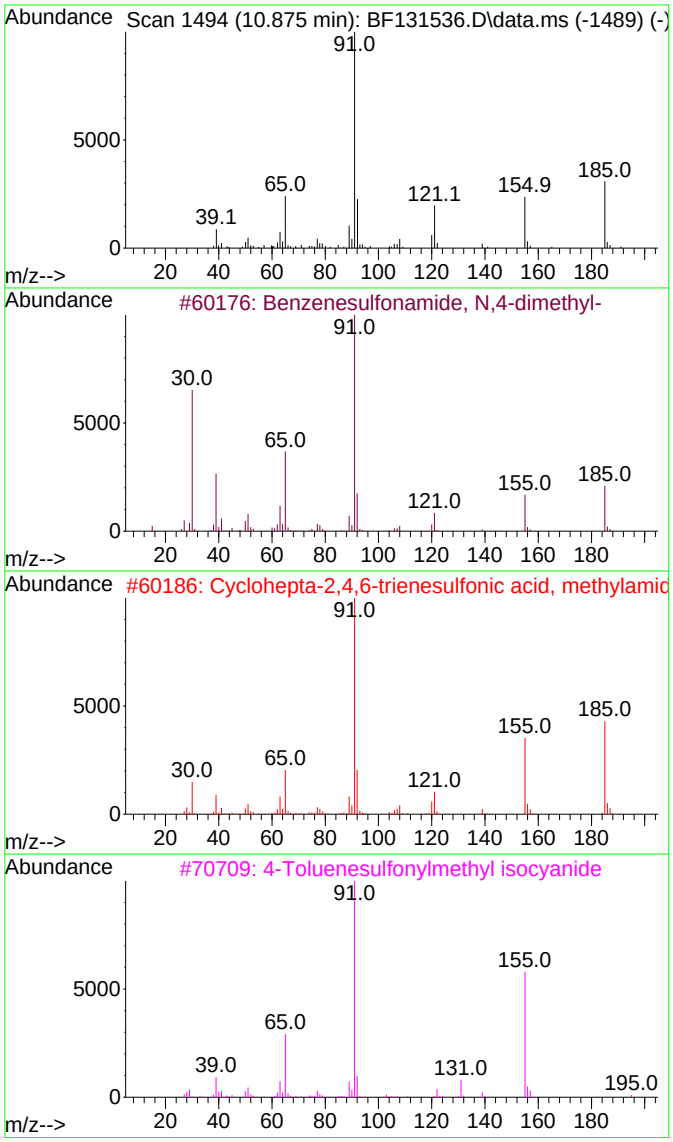
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

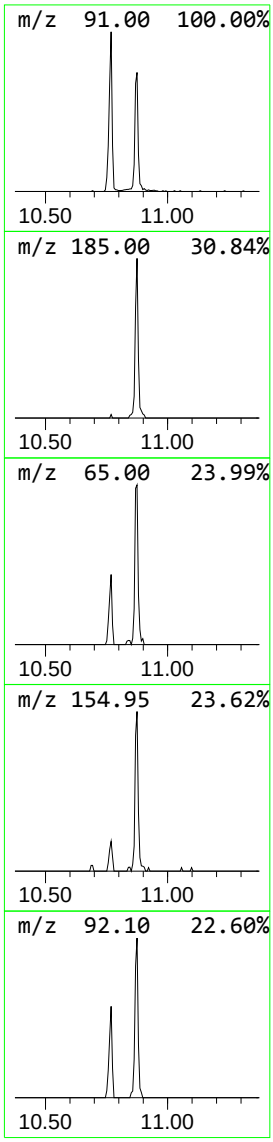
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 7 Benzenesulfonamide, N,4-dim... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.875 | 2.27 ng | 96373 | Phenanthrene-d10 | 11.469 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzenesulfonamide, N,4-dimethyl- | 185 | C8H11NO2S | 000640-61-9 | 94 |
| 2 | Cyclohepta-2,4,6-trienesulfonic ... | 185 | C8H11NO2S | 1000187-28-7 | 59 |
| 3 | 4-Toluenesulfonylmethyl isocyanide | 195 | C9H9NO2S | 036635-61-7 | 47 |
| 4 | p-Toluenesulfonylacetonitrile | 195 | C9H9NO2S | 005697-44-9 | 43 |
| 5 | (O-p-Tosylisonitroso)malononitrile | 249 | C10H7N3O3S | 020893-01-0 | 43 |



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Sample : N5870-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
ML-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

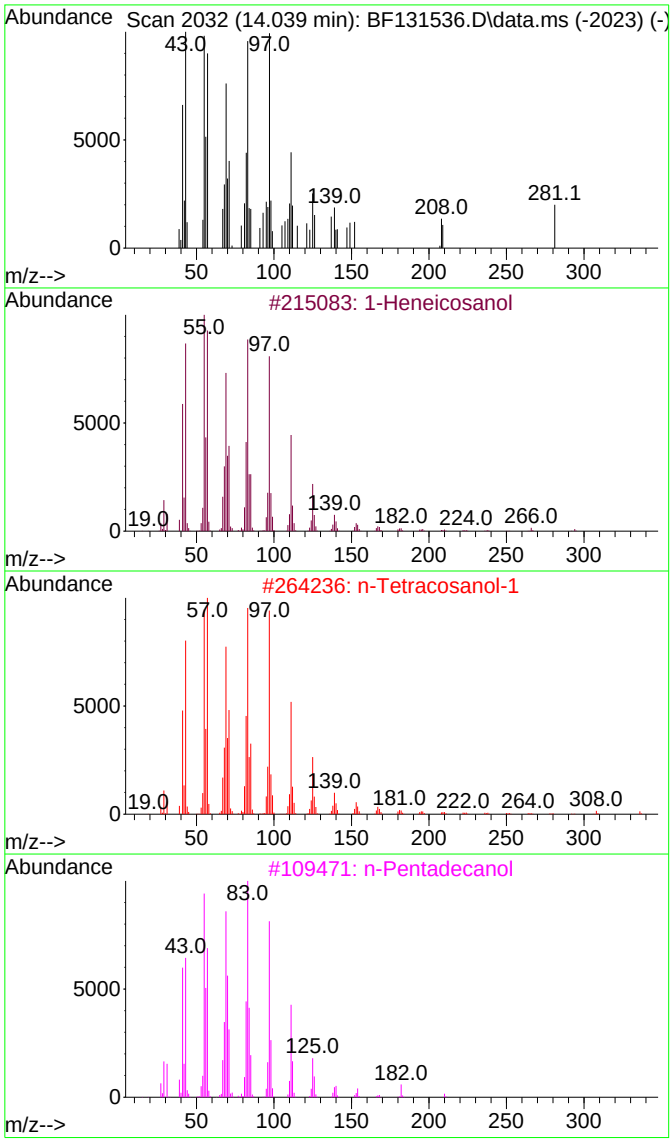
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

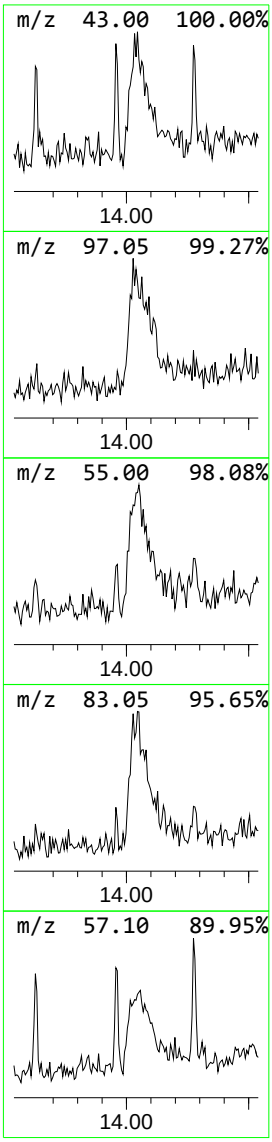
**********

Peak Number 8 1-Heneicosanol Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.039 | 4.10 ng | 112820 | Chrysene-d12 | 14.121 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 83 |
| 2 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 83 |
| 3 | n-Pentadecanol | 228 | C15H32O | 000629-76-5 | 83 |
| 4 | 1-Hexadecanol | 242 | C16H34O | 036653-82-4 | 80 |
| 5 | n-Heptadecanol-1 | 256 | C17H36O | 001454-85-9 | 74 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120622\
Data File : BF131536.D
Acq On : 06 Dec 2022 20:00
Operator : CG\JU
Sample : N5870-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
ML-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120522.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 |
| Butane, 2-metho... | 2.246 | 24.4 | ng | 605212 | 1 | 6.922 | 496046 | 20.0 |
| Propane, 1,1-di... | 2.358 | 2.0 | ng | 49832 | 1 | 6.922 | 496046 | 20.0 |
| 2-Pentanone, 4-... | 5.151 | 33.6 | ng | 833234 | 1 | 6.922 | 496046 | 20.0 |
| 2-Pentanone, 4-... | 5.934 | 2.5 | ng | 63350 | 1 | 6.922 | 496046 | 20.0 |
| Di-tert-butyl d... | 7.745 | 4.9 | ng | 155036 | 2 | 8.210 | 628059 | 20.0 |
| Benzophenone | 10.692 | 3.2 | ng | 124981 | 3 | 9.975 | 786309 | 20.0 |
| Benzenesulfonam... | 10.875 | 2.3 | ng | 96373 | 4 | 11.469 | 847817 | 20.0 |
| 1-Heneicosanol | 14.039 | 4.1 | ng | 112820 | 5 | 14.121 | 550433 | 20.0 |