LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061022\
Data File : BF128761.D
Acq On : 10 Jun 2022 16:18
Operator : CG\JU
Sample : N3286-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-6D

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-BF060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128761.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 3.128 | 136 | 143 | 146 | rBV | 43407 | 77676 | 2.67% | 0.549% |
| 2 | 3.169 | 146 | 150 | 159 | rVB | 86074 | 144738 | 4.98% | 1.023% |
| 3 | 3.652 | 224 | 232 | 239 | rBV | 135595 | 206545 | 7.10% | 1.459% |
| 4 | 4.352 | 348 | 351 | 355 | rVB | 61892 | 67725 | 2.33% | 0.478% |
| 5 | 4.922 | 442 | 448 | 453 | rBV | 38946 | 46152 | 1.59% | 0.326% |
| 6 | 5.010 | 460 | 463 | 466 | rBV | 49481 | 50044 | 1.72% | 0.354% |
| 7 | 5.063 | 470 | 472 | 475 | rBV2 | 50716 | 55775 | 1.92% | 0.394% |
| 8 | 5.281 | 505 | 509 | 514 | rVB3 | 38082 | 42133 | 1.45% | 0.298% |
| 9 | 5.451 | 535 | 538 | 544 | rBV | 758302 | 706462 | 24.29% | 4.991% |
| 10 | 6.457 | 706 | 709 | 718 | rVB | 437170 | 423651 | 14.56% | 2.993% |
| 11 | 6.798 | 763 | 767 | 771 | rVB | 540047 | 437203 | 15.03% | 3.089% |
| 12 | 6.981 | 794 | 798 | 801 | rVB | 121467 | 116955 | 4.02% | 0.826% |
| 13 | 7.369 | 853 | 864 | 867 | rBV | 1405211 | 1582522 | 54.41% | 11.180% |
| 14 | 7.757 | 926 | 930 | 937 | rBV2 | 26042 | 35939 | 1.24% | 0.254% |
| 15 | 8.087 | 981 | 986 | 989 | rBV | 565917 | 575321 | 19.78% | 4.065% |
| 16 | 9.163 | 1163 | 1169 | 1172 | rBV | 3013530 | 2908746 | 100.00% | 20.550% |
| 17 | 9.839 | 1278 | 1284 | 1288 | rBV | 813343 | 695000 | 23.89% | 4.910% |
| 18 | 10.633 | 1413 | 1419 | 1423 | rBV | 1688622 | 1696609 | 58.33% | 11.986% |
| 19 | 11.328 | 1533 | 1537 | 1541 | rVB | 862969 | 705537 | 24.26% | 4.984% |
| 20 | 11.863 | 1624 | 1628 | 1634 | rBV5 | 22687 | 33377 | 1.15% | 0.236% |
| 21 | 12.922 | 1803 | 1808 | 1811 | rBV | 2719862 | 2387107 | 82.07% | 16.864% |
| 22 | 13.839 | 1960 | 1964 | 1972 | rVB4 | 25602 | 45123 | 1.55% | 0.319% |
| 23 | 13.974 | 1981 | 1987 | 1990 | rBV | 443904 | 400747 | 13.78% | 2.831% |
| 24 | 14.069 | 1997 | 2003 | 2007 | rBV | 196963 | 223643 | 7.69% | 1.580% |
| 25 | 15.433 | 2230 | 2235 | 2244 | rVB | 332805 | 425852 | 14.64% | 3.009% |
| 26 | 15.892 | 2308 | 2313 | 2318 | rVB3 | 20789 | 33500 | 1.15% | 0.237% |
| 27 | 16.386 | 2393 | 2397 | 2402 | rVB4 | 19865 | 30629 | 1.05% | 0.216% |

Sum of corrected areas: 14154711

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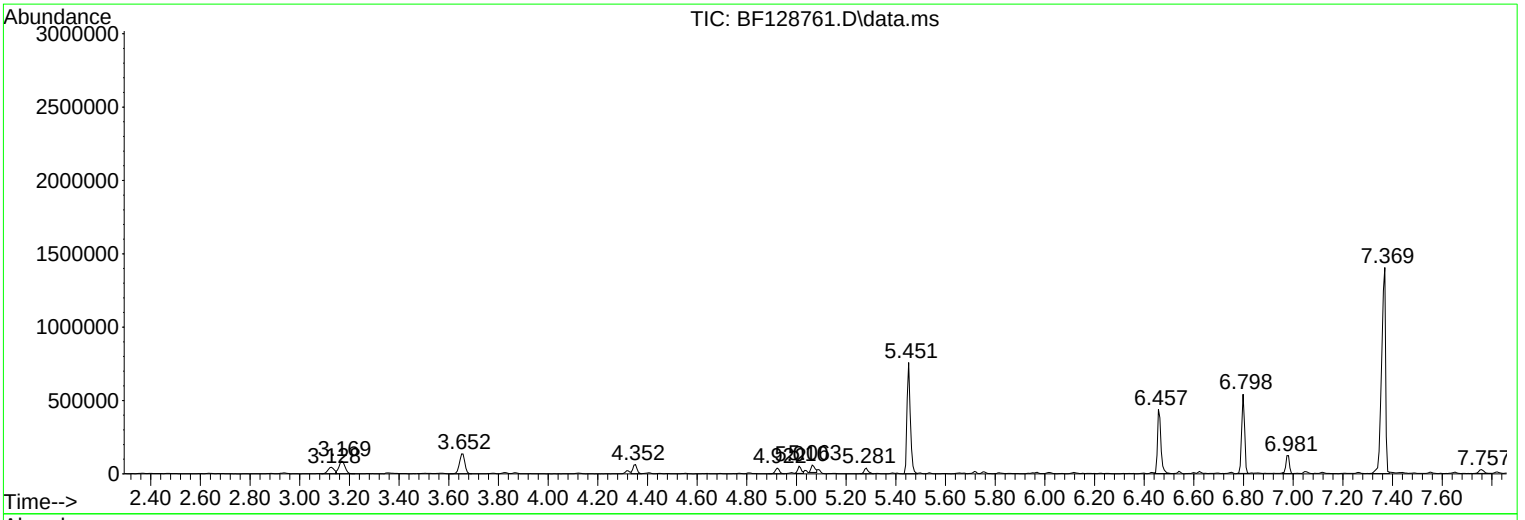
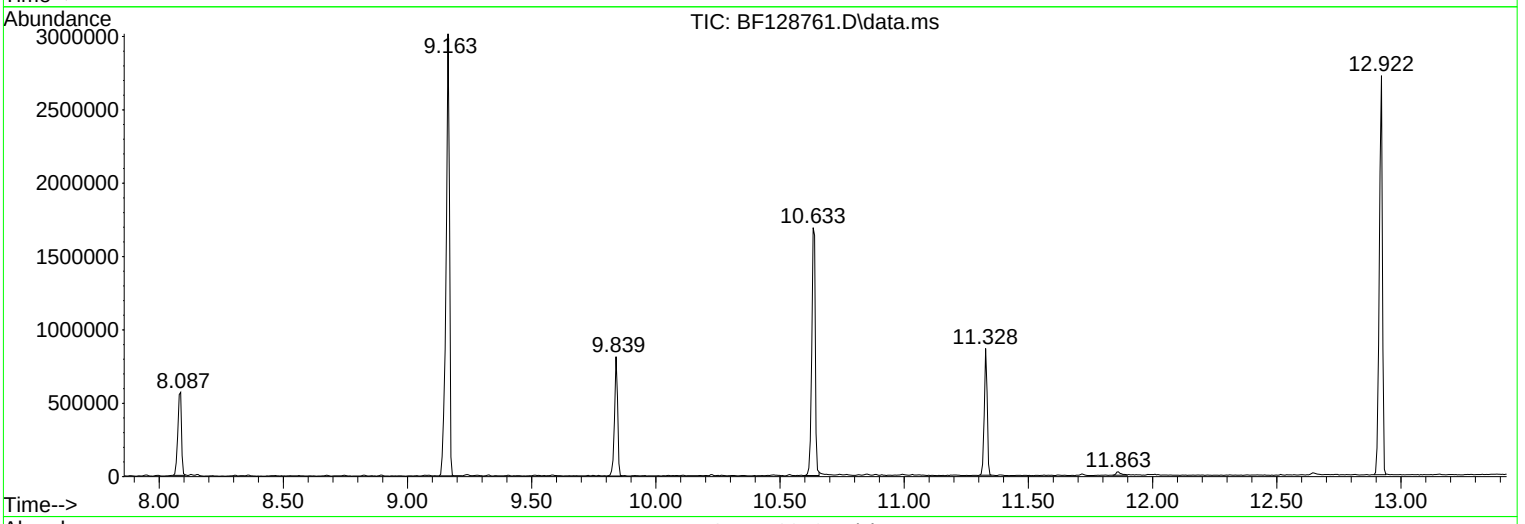
Misc :
ALS Vial : 8 Sample Multiplier: 1

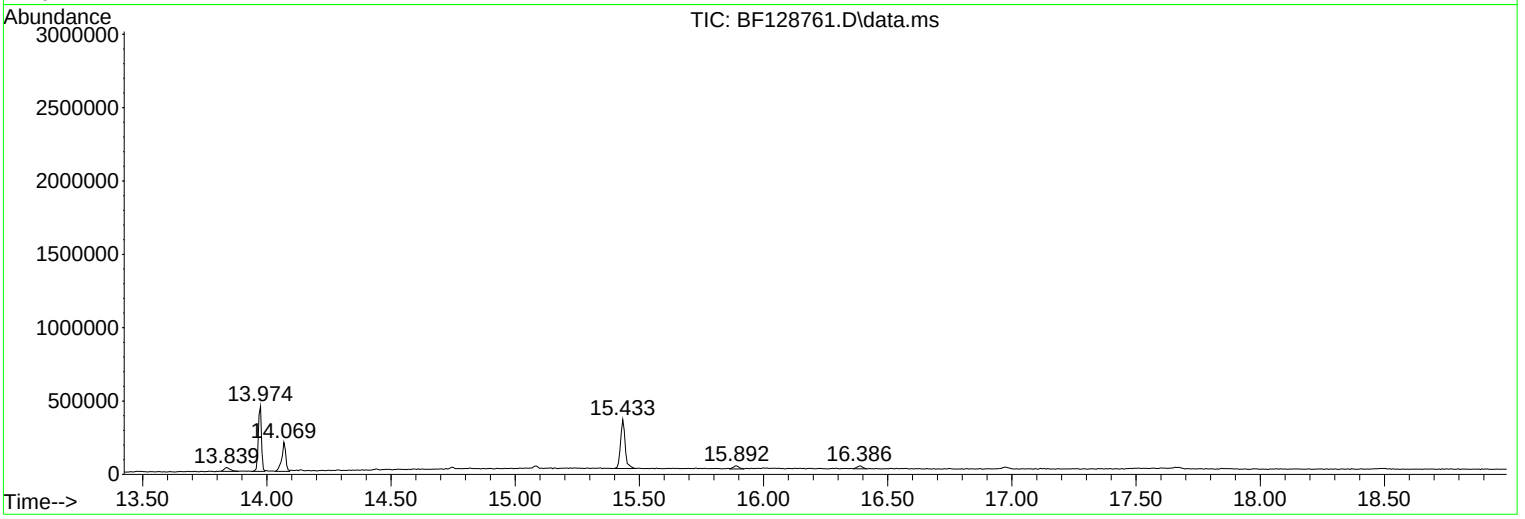
**Instrument :**
BNA_F
**ClientSampleId :**
MW-6D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061022\
Data File : BF128761.D
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Operator : CG\JU
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**Instrument :**
BNA_F
**ClientSampleId :**
MW-6D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

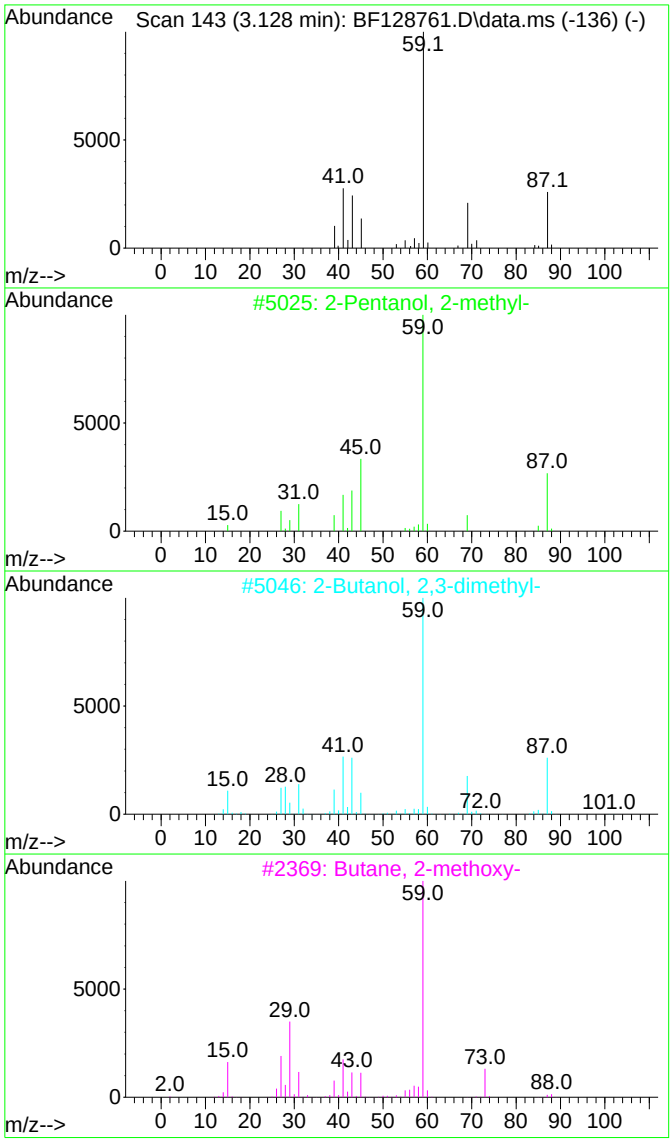
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

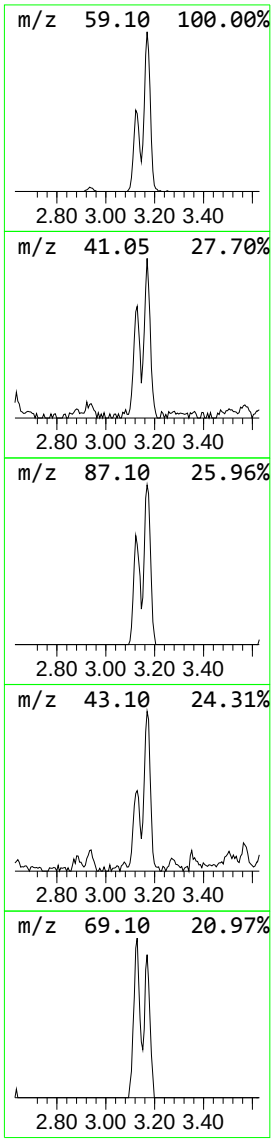
**********

Peak Number 1 2-Pentanol, 2-methyl- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.128 | 3.55 ng | 77676 | 1,4-Dichlorobenzene-d4 | 6.798 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanol, 2-methyl- | 102 | C6H14O | 000590-36-3 | 78 |
| 2 | 2-Butanol, 2,3-dimethyl- | 102 | C6H14O | 000594-60-5 | 74 |
| 3 | Butane, 2-methoxy- | 88 | C5H12O | 006795-87-5 | 45 |
| 4 | 3-Pentanol, 2,2-dimethyl- | 116 | C7H16O | 003970-62-5 | 40 |
| 5 | 3-Heptanol | 116 | C7H16O | 000589-82-2 | 40 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061022\
Data File : BF128761.D
Acq On : 10 Jun 2022 16:18
Operator : CG\JU
Sample : N3286-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
MW-6D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

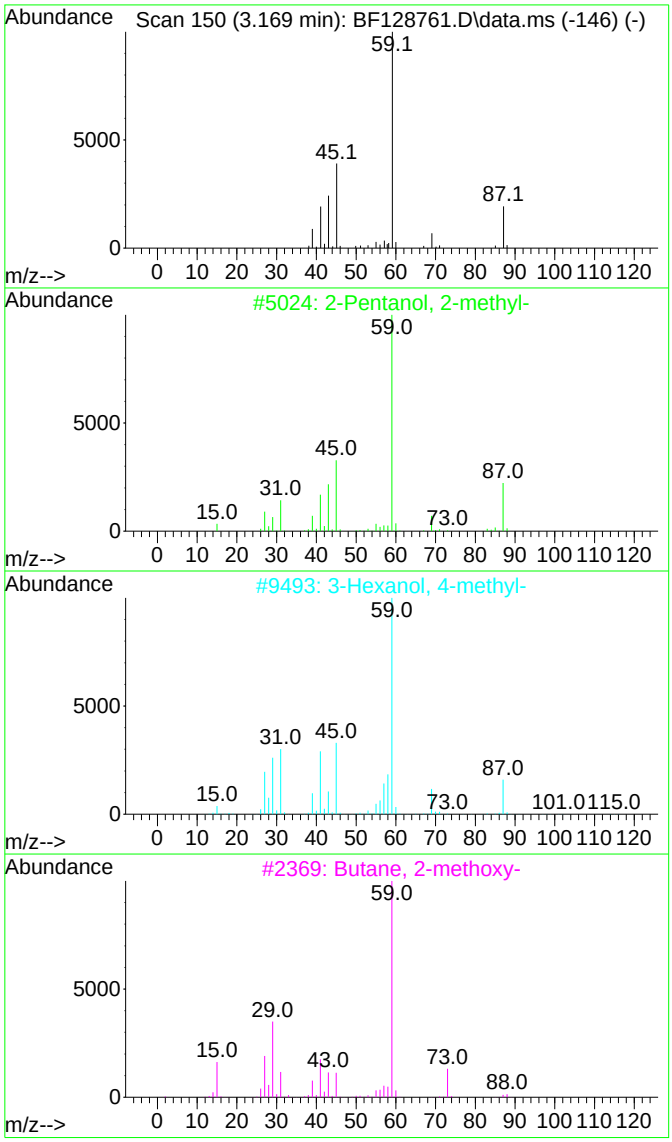
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

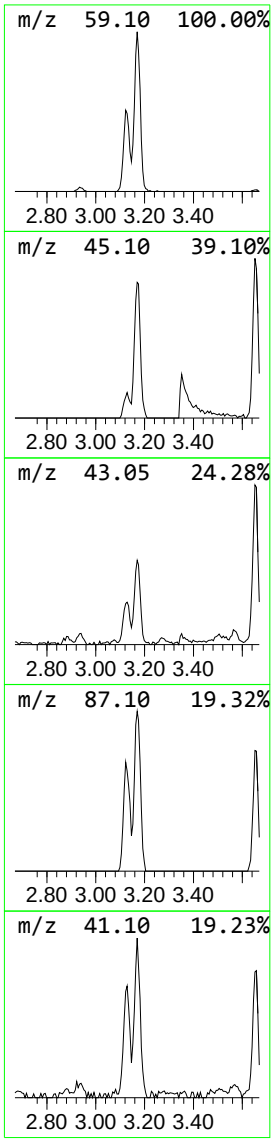
**********

Peak Number 2 unknown3.169 Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.169 | 6.62 ng | 144738 | 1,4-Dichlorobenzene-d4 | 6.798 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanol, 2-methyl- | 102 | C6H14O | 000590-36-3 | 72 |
| 2 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 40 |
| 3 | Butane, 2-methoxy- | 88 | C5H12O | 006795-87-5 | 9 |
| 4 | Acetaldehyde, O-ethyloxime- | 87 | C4H9NO | 1000288-34-6 | 9 |
| 5 | Thiocyanic acid, ethyl ester | 87 | C3H5NS | 000542-90-5 | 9 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061022\
Data File : BF128761.D
Acq On : 10 Jun 2022 16:18
Operator : CG\JU
Sample : N3286-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
MW-6D

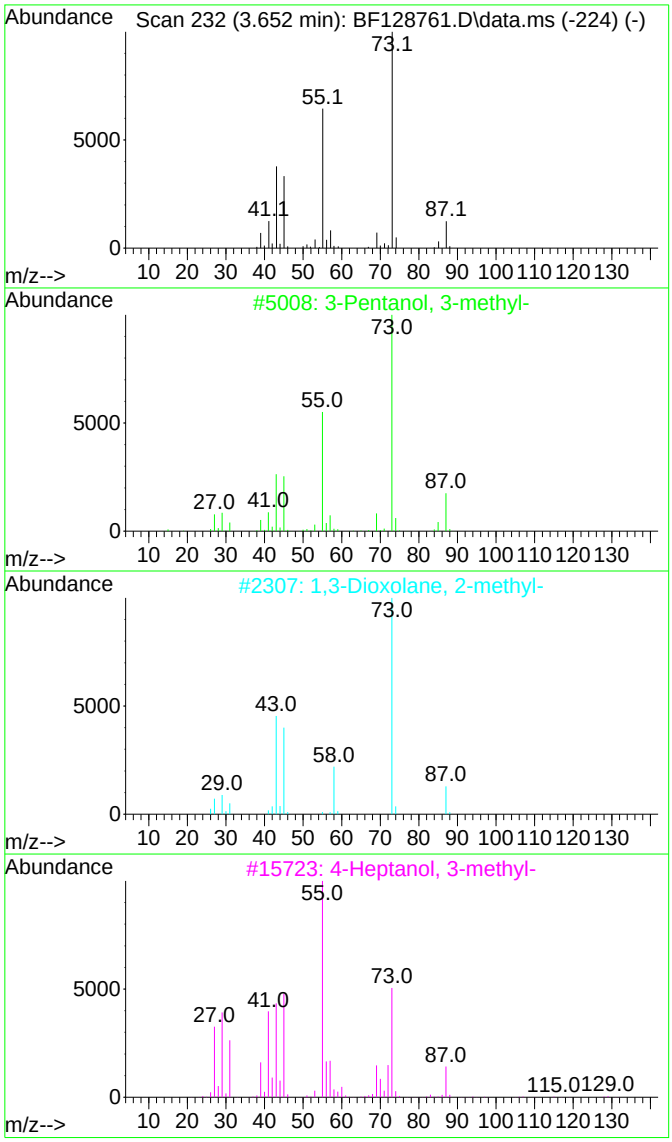
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

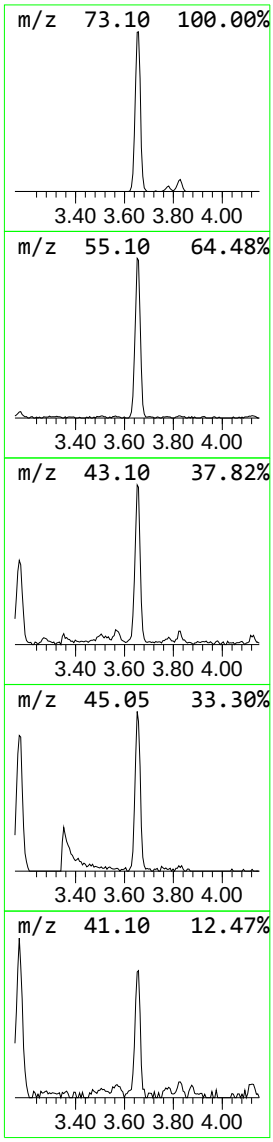
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 3 3-Pentanol, 3-methyl- Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.652 | 9.45 ng | 206545 | 1,4-Dichlorobenzene-d4 | 6.798 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Pentanol, 3-methyl- | 102 | C6H14O | 000077-74-7 | 72 |
| 2 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 50 |
| 3 | 4-Heptanol, 3-methyl- | 130 | C8H18O | 001838-73-9 | 39 |
| 4 | 1,3-Dioxolane, 2-(1-bromoethyl)- | 180 | C5H9BrO2 | 005267-73-2 | 38 |
| 5 | 1,3-Dioxolane, 2-(1-methylethyl)- | 116 | C6H12O2 | 000822-83-3 | 33 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061022\
Data File : BF128761.D
Acq On : 10 Jun 2022 16:18
Operator : CG\JU
Sample : N3286-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
MW-6D

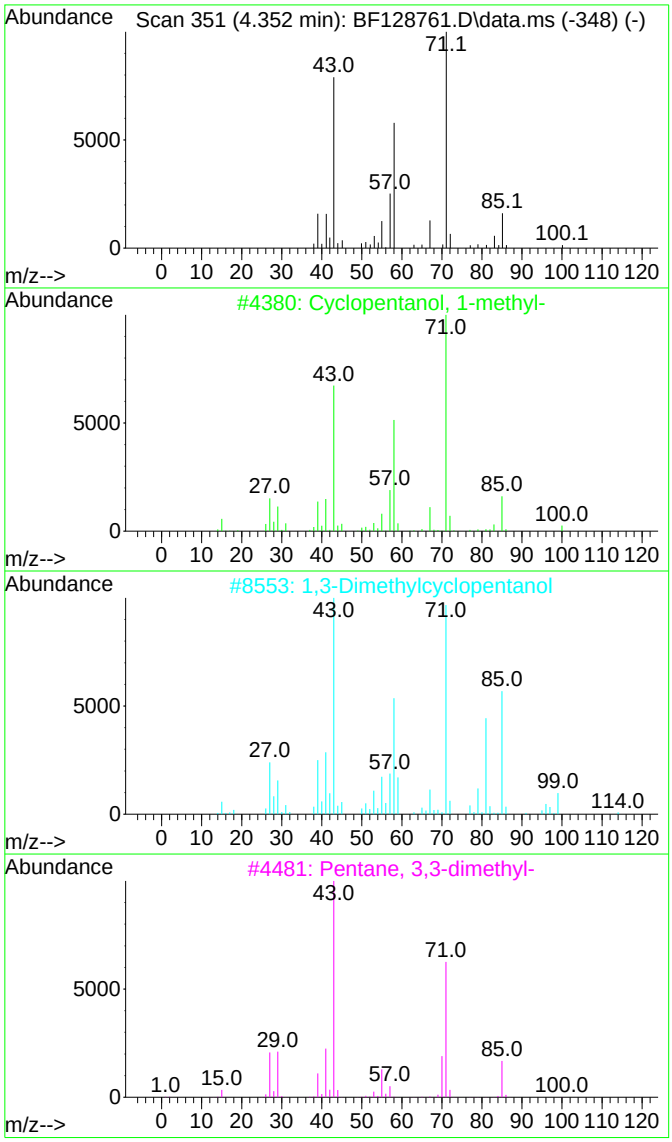
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

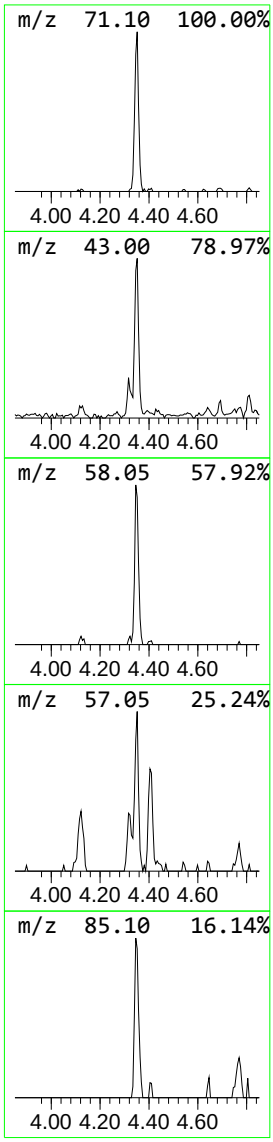
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 4 Cyclopentanol, 1-methyl- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.352 | 3.10 ng | 67725 | 1,4-Dichlorobenzene-d4 | 6.798 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Cyclopentanol, 1-methyl- | 100 | C6H12O | 001462-03-9 | 83 |
| 2 | 1,3-Dimethylcyclopentanol | 114 | C7H14O | 019550-46-0 | 78 |
| 3 | Pentane, 3,3-dimethyl- | 100 | C7H16 | 000562-49-2 | 50 |
| 4 | Pentane, 3-bromo- | 150 | C5H11Br | 001809-10-5 | 47 |
| 5 | 1-Penten-3-ol, 2-methyl- | 100 | C6H12O | 002088-07-5 | 47 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061022\
Data File : BF128761.D
Acq On : 10 Jun 2022 16:18
Operator : CG\JU
Sample : N3286-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
MW-6D

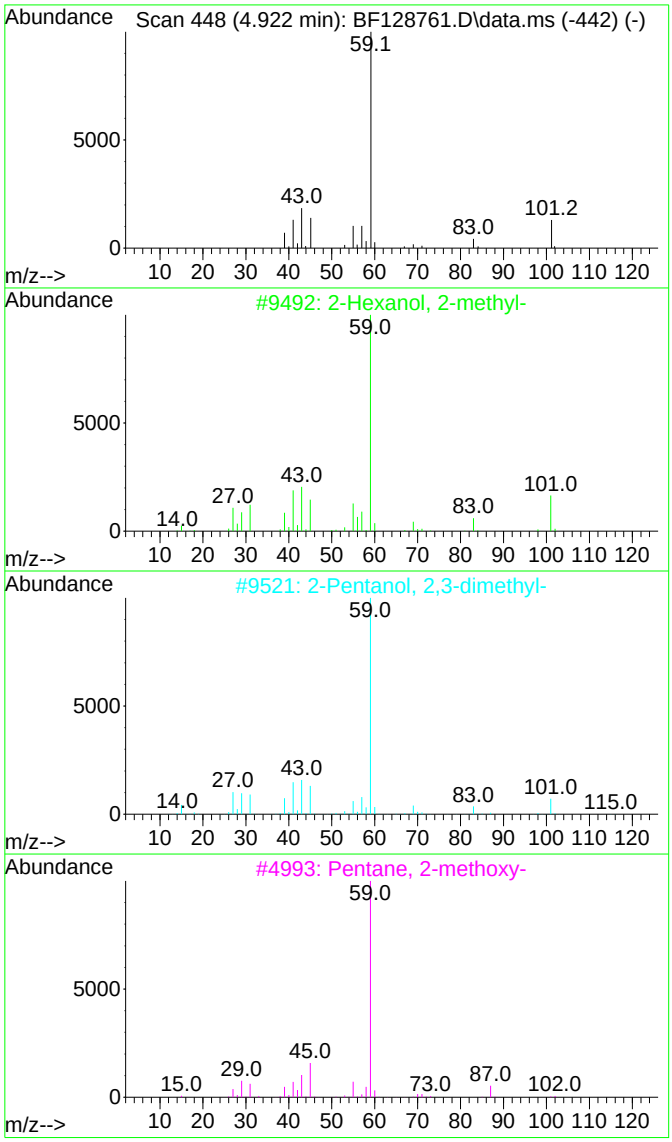
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

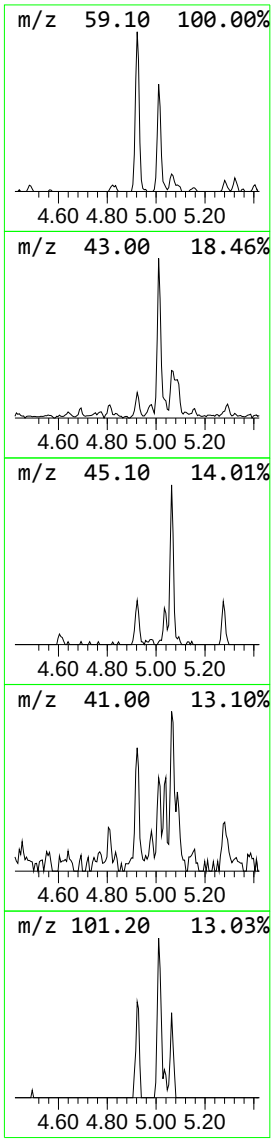
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 5 2-Hexanol, 2-methyl- Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.922 | 2.11 ng | 46152 | 1,4-Dichlorobenzene-d4 | 6.798 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 83 |
| 2 | 2-Pentanol, 2,3-dimethyl- | 116 | C7H16O | 004911-70-0 | 78 |
| 3 | Pentane, 2-methoxy- | 102 | C6H14O | 006795-88-6 | 59 |
| 4 | 3-Hexanol, 4-ethyl- | 130 | C8H18O | 019780-44-0 | 56 |
| 5 | Ethanol, pentamethyl- | 116 | C7H16O | 000594-83-2 | 56 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061022\
Data File : BF128761.D
Acq On : 10 Jun 2022 16:18
Operator : CG\JU
Sample : N3286-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
MW-6D

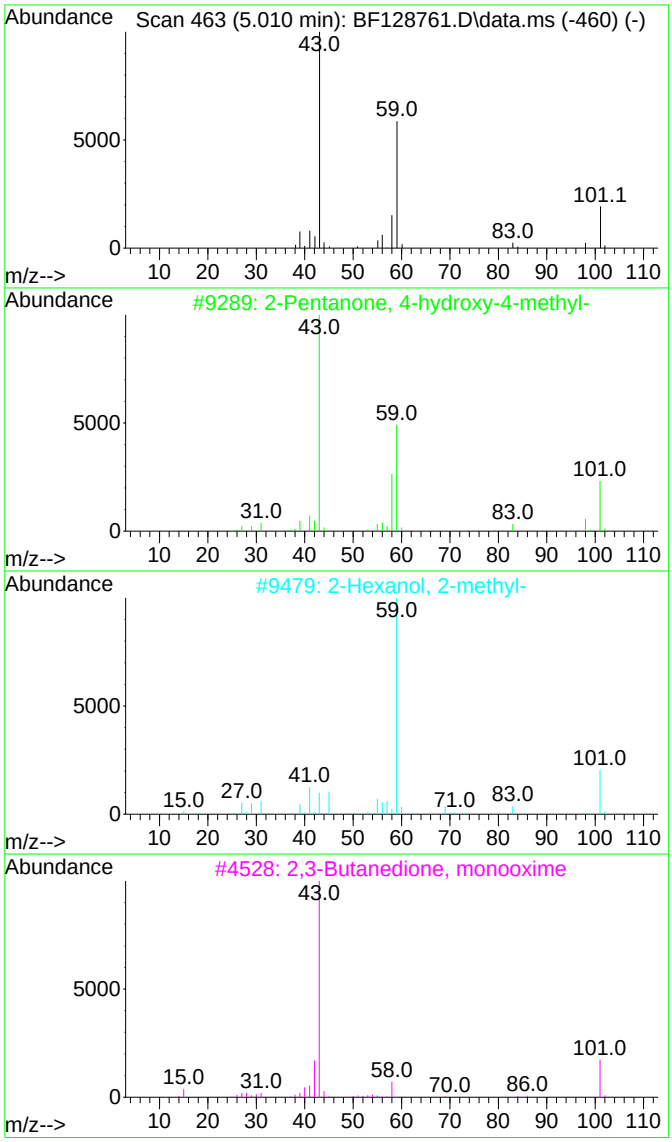
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

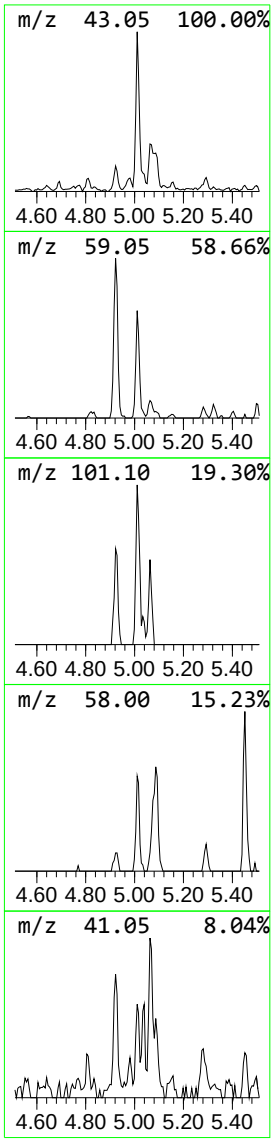
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.010 | 2.29 ng | 50044 | 1,4-Dichlorobenzene-d4 | 6.798 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 72 |
| 2 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 28 |
| 3 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 25 |
| 4 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23 |
| 5 | 4-Penten-2-one, 4-methyl- | 98 | C6H10O | 003744-02-3 | 10 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061022\
Data File : BF128761.D
Acq On : 10 Jun 2022 16:18
Operator : CG\JU
Sample : N3286-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
MW-6D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

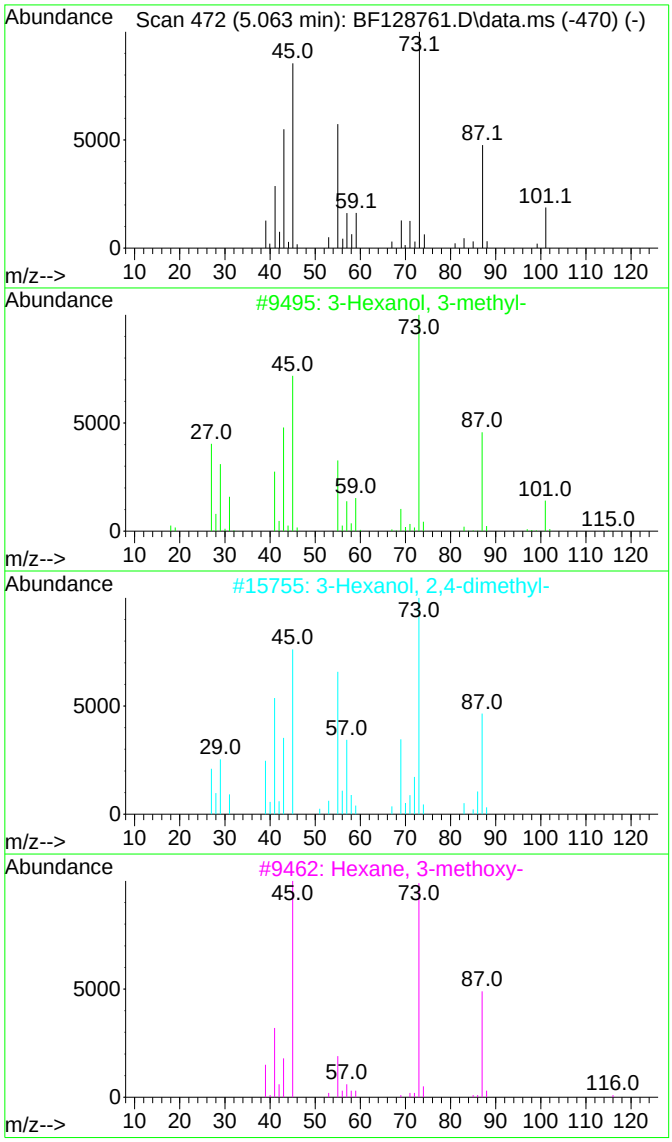
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

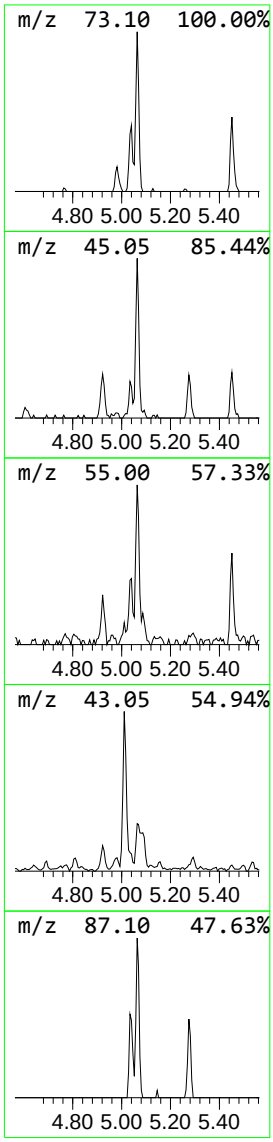
**********

Peak Number 7 3-Hexanol, 3-methyl- Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.063 | 2.55 ng | 55775 | 1,4-Dichlorobenzene-d4 | 6.798 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Hexanol, 3-methyl- | 116 | C7H16O | 000597-96-6 | 86 |
| 2 | 3-Hexanol, 2,4-dimethyl- | 130 | C8H18O | 013432-25-2 | 64 |
| 3 | Hexane, 3-methoxy- | 116 | C7H16O | 054658-01-4 | 59 |
| 4 | 3-Pentanol, 2,3-dimethyl- | 116 | C7H16O | 000595-41-5 | 50 |
| 5 | 3-Hexanone, 5-hydroxy-2-methyl- | 130 | C7H14O2 | 059357-07-2 | 50 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061022\
Data File : BF128761.D
Acq On : 10 Jun 2022 16:18
Operator : CG\JU
Sample : N3286-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
MW-6D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

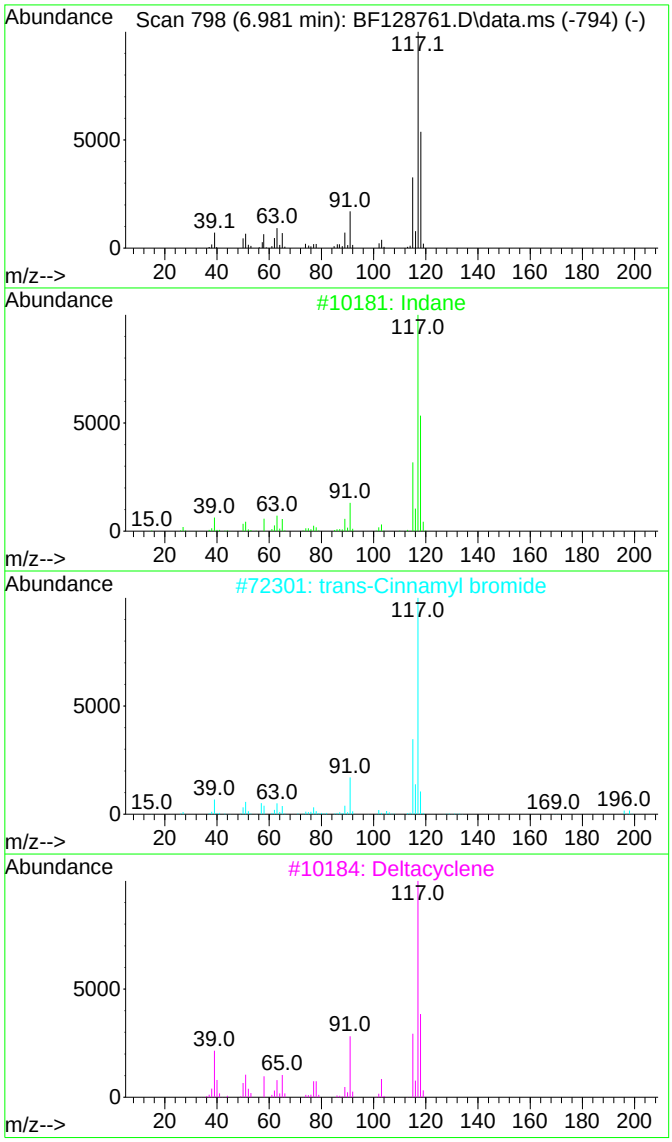
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

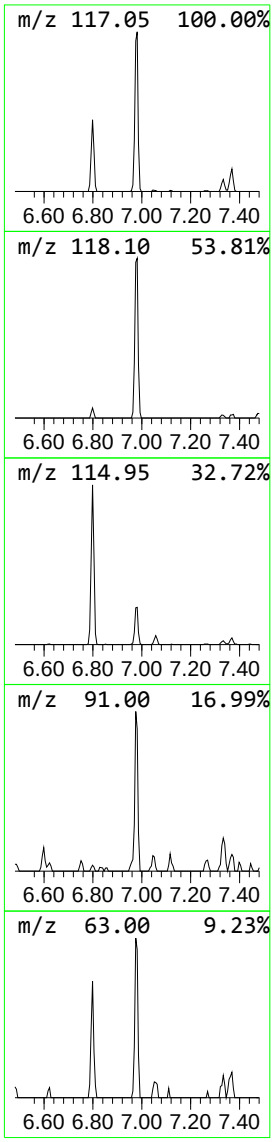
**********

Peak Number 8 Indane Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.981 | 5.35 ng | 116955 | 1,4-Dichlorobenzene-d4 | 6.798 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Indane | 118 | C9H10 | 000496-11-7 | 87 |
| 2 | trans-Cinnamyl bromide | 196 | C9H9Br | 026146-77-0 | 64 |
| 3 | Deltacyclene | 118 | C9H10 | 007785-10-6 | 59 |
| 4 | Benzene, 1-propenyl- | 118 | C9H10 | 000637-50-3 | 53 |
| 5 | Benzene, cyclopropyl- | 118 | C9H10 | 000873-49-4 | 53 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061022\
Data File : BF128761.D
Acq On : 10 Jun 2022 16:18
Operator : CG\JU
Sample : N3286-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
MW-6D

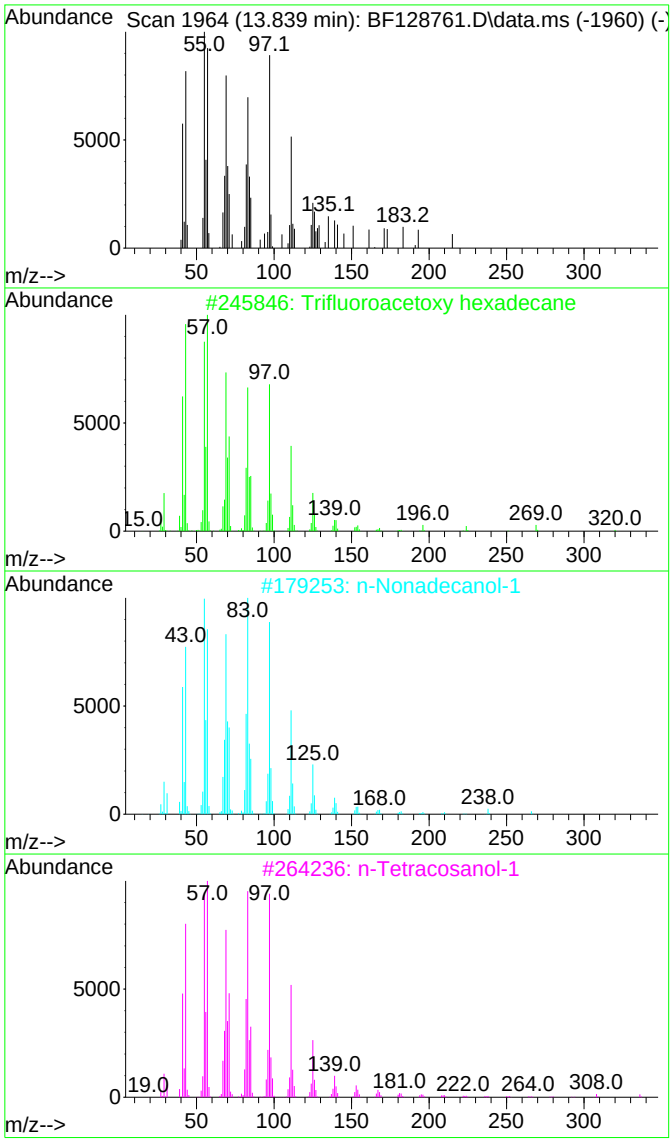
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

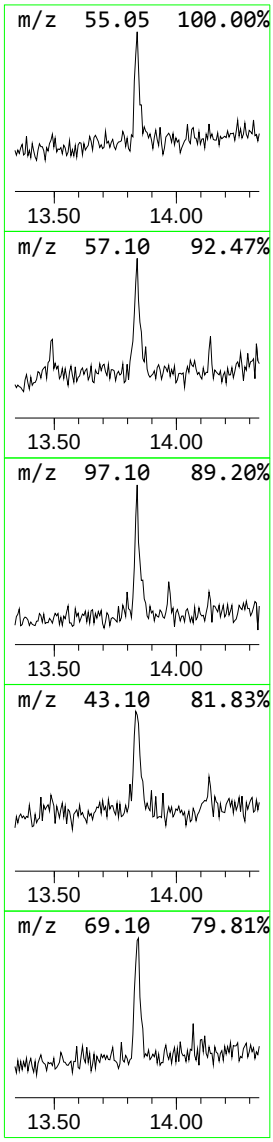
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 9 Trifluoroacetoxy hexadecane Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.839 | 2.25 ng | 45123 | Chrysene-d12 | 13.974 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3 | 91 |
| 2 | n-Nonadecanol-1 | 284 | C19H40O | 001454-84-8 | 91 |
| 3 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 90 |
| 4 | Behenic alcohol | 326 | C22H46O | 000661-19-8 | 90 |
| 5 | 1-Hexacosene | 364 | C26H52 | 018835-33-1 | 87 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061022\
Data File : BF128761.D
Acq On : 10 Jun 2022 16:18
Operator : CG\JU
Sample : N3286-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
MW-6D

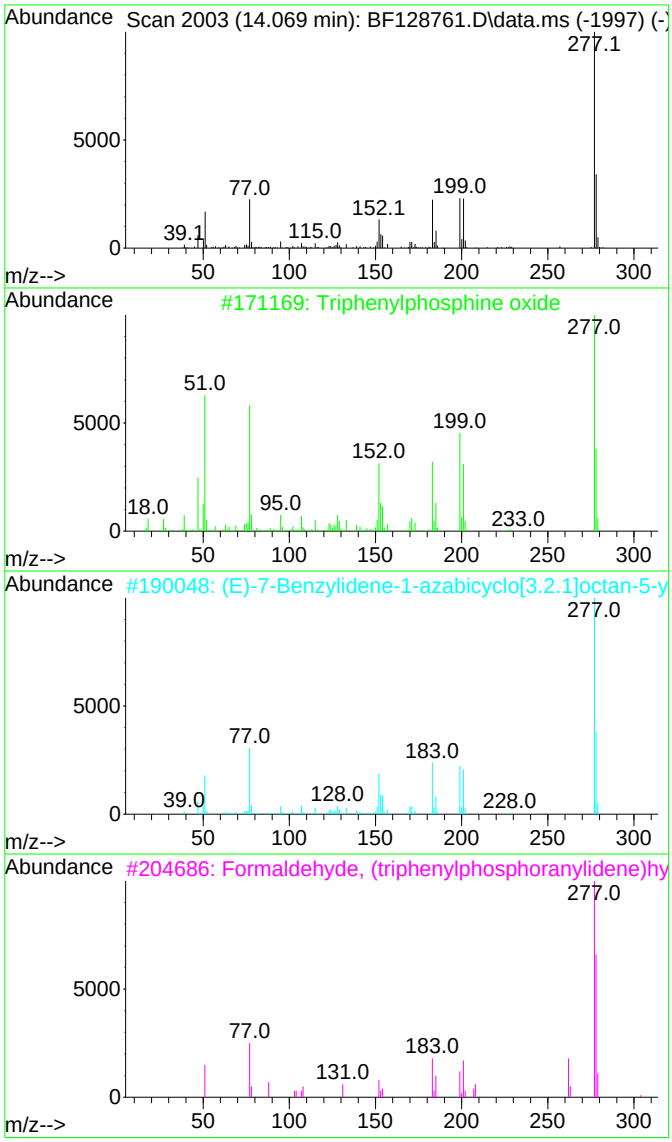
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

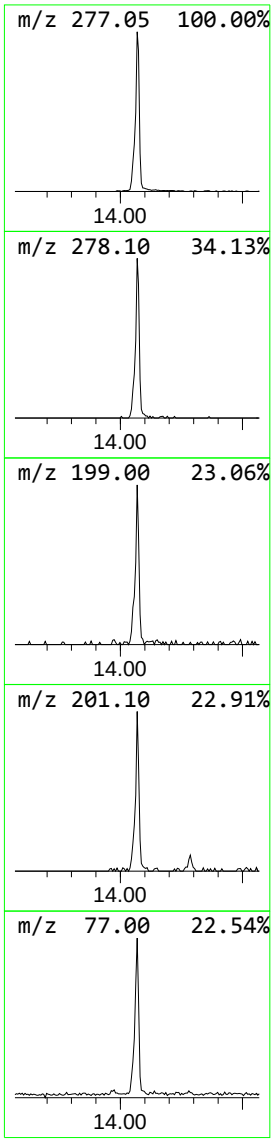
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

**********
Peak Number 10 Triphenylphosphine oxide Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.069 | 11.16 ng | 223643 | Chrysene-d12 | 13.974 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Triphenylphosphine oxide | 278 | C18H15OP | 000791-28-6 | 99 |
| 2 | (E)-7-Benzylidene-1-azabicyclo[3... | 293 | C15H19NO3S | 1000483-83-4 | 87 |
| 3 | Formaldehyde, (triphenylphosphor... | 304 | C19H17N2P | 015990-54-2 | 42 |
| 4 | Cobalt,(.eta.<5>-2,4-cyclopentad... | 277 | C16H15BCo | 036682-12-9 | 32 |
| 5 | Vanadium, cycloheptatrienyl-(pen... | 277 | C17H22V | 1000155-20-5 | 23 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061022\
Data File : BF128761.D
Acq On : 10 Jun 2022 16:18
Operator : CG\JU
Sample : N3286-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
MW-6D

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.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 |
| 2-Pentanol, 2-m... | 3.128 | 3.5 | ng | 77676 | 1 | 6.798 | 437203 | 20.0 |
| unknown3.169 | 3.169 | 6.6 | ng | 144738 | 1 | 6.798 | 437203 | 20.0 |
| 3-Pentanol, 3-m... | 3.652 | 9.4 | ng | 206545 | 1 | 6.798 | 437203 | 20.0 |
| Cyclopentanol, ... | 4.352 | 3.1 | ng | 67725 | 1 | 6.798 | 437203 | 20.0 |
| 2-Hexanol, 2-me... | 4.922 | 2.1 | ng | 46152 | 1 | 6.798 | 437203 | 20.0 |
| 2-Pentanone, 4-... | 5.010 | 2.3 | ng | 50044 | 1 | 6.798 | 437203 | 20.0 |
| 3-Hexanol, 3-me... | 5.063 | 2.5 | ng | 55775 | 1 | 6.798 | 437203 | 20.0 |
| Indane | 6.981 | 5.3 | ng | 116955 | 1 | 6.798 | 437203 | 20.0 |
| Trifluoroacetox... | 13.839 | 2.3 | ng | 45123 | 5 | 13.974 | 400747 | 20.0 |
| Triphenylphosph... | 14.069 | 11.2 | ng | 223643 | 5 | 13.974 | 400747 | 20.0 |