LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092624\
Data File : BF139564.D
Acq On : 26 Sep 2024 23:48
Operator : RC/JU
Sample : P4198-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP1-5-WC-1

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-BF091324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139564.D\data.ms

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.157 | 3 | 11 | 17 | rVB | 1370844 | 2151418 | 100.00% | 16.114% |
| 2 | 3.375 | 213 | 218 | 242 | rBV | 19338 | 63897 | 2.97% | 0.479% |
| 3 | 5.087 | 499 | 509 | 517 | rBV | 72839 | 111276 | 5.17% | 0.833% |
| 4 | 5.492 | 572 | 578 | 583 | rBV | 1068408 | 1361815 | 63.30% | 10.200% |
| 5 | 6.504 | 744 | 750 | 755 | rBV | 1132366 | 1478271 | 68.71% | 11.072% |
| 6 | 6.875 | 808 | 813 | 818 | rBV | 356510 | 425000 | 19.75% | 3.183% |
| 7 | 7.434 | 903 | 908 | 913 | rBV | 687766 | 875164 | 40.68% | 6.555% |
| 8 | 7.692 | 947 | 952 | 956 | rBV | 17896 | 23835 | 1.11% | 0.179% |
| 9 | 8.157 | 1026 | 1031 | 1036 | rBV | 437951 | 534393 | 24.84% | 4.003% |
| 10 | 8.469 | 1079 | 1084 | 1098 | rBV | 41930 | 61085 | 2.84% | 0.458% |
| 11 | 9.228 | 1208 | 1213 | 1222 | rBV | 1162794 | 1514198 | 70.38% | 11.341% |
| 12 | 9.622 | 1276 | 1280 | 1283 | rBV3 | 14330 | 22467 | 1.04% | 0.168% |
| 13 | 9.775 | 1302 | 1306 | 1309 | rBV3 | 24203 | 35831 | 1.67% | 0.268% |
| 14 | 9.822 | 1310 | 1314 | 1317 | rVB | 31273 | 43597 | 2.03% | 0.327% |
| 15 | 9.910 | 1323 | 1329 | 1334 | rBV | 480124 | 610870 | 28.39% | 4.575% |
| 16 | 10.004 | 1342 | 1345 | 1351 | rVB3 | 26612 | 39836 | 1.85% | 0.298% |
| 17 | 10.316 | 1395 | 1398 | 1402 | rBV2 | 51136 | 61085 | 2.84% | 0.458% |
| 18 | 10.698 | 1458 | 1463 | 1469 | rBV | 720678 | 953317 | 44.31% | 7.140% |
| 19 | 11.398 | 1578 | 1582 | 1591 | rVB | 491443 | 608522 | 28.28% | 4.558% |
| 20 | 11.921 | 1668 | 1671 | 1676 | rBV3 | 50930 | 71264 | 3.31% | 0.534% |
| 21 | 12.980 | 1846 | 1851 | 1859 | rVB | 1170030 | 1484601 | 69.01% | 11.120% |
| 22 | 14.033 | 2025 | 2030 | 2042 | rVB | 320683 | 420911 | 19.56% | 3.153% |
| 23 | 15.504 | 2274 | 2280 | 2291 | rBV | 246426 | 398660 | 18.53% | 2.986% |

Sum of corrected areas: 13351313

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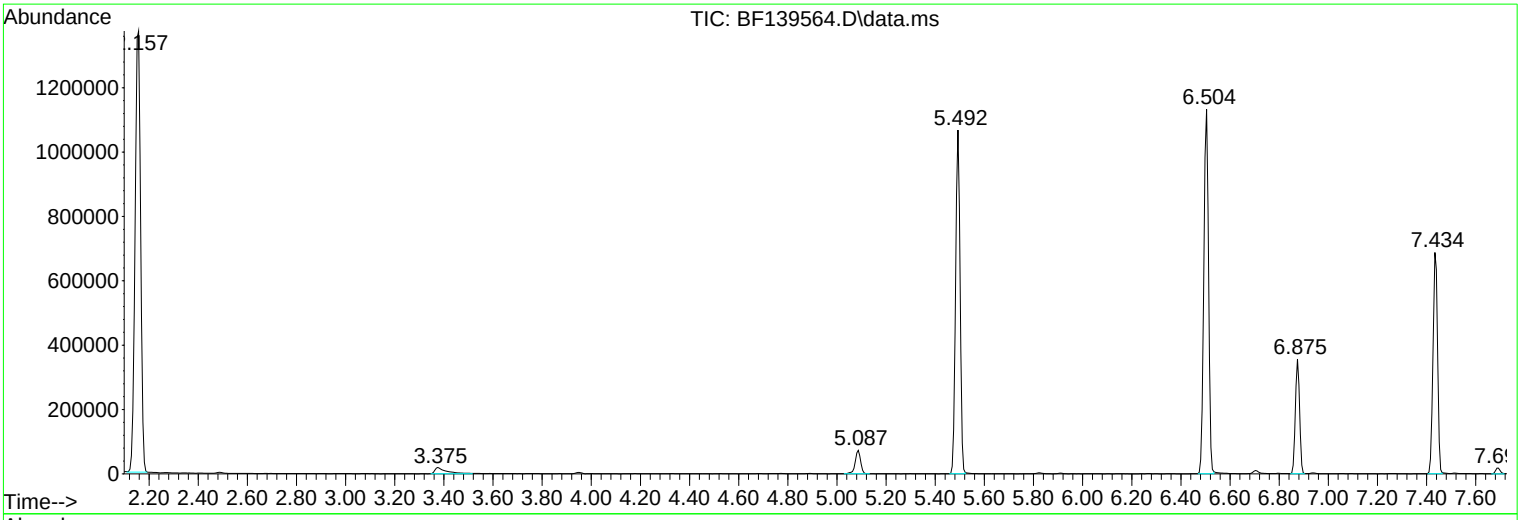
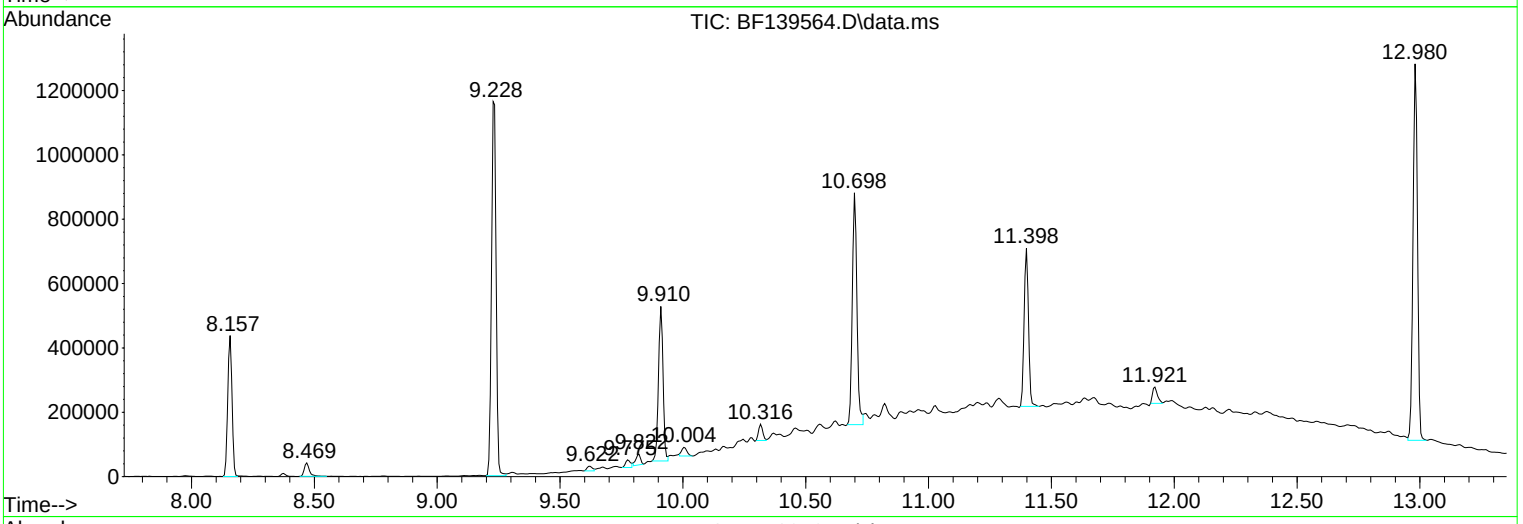
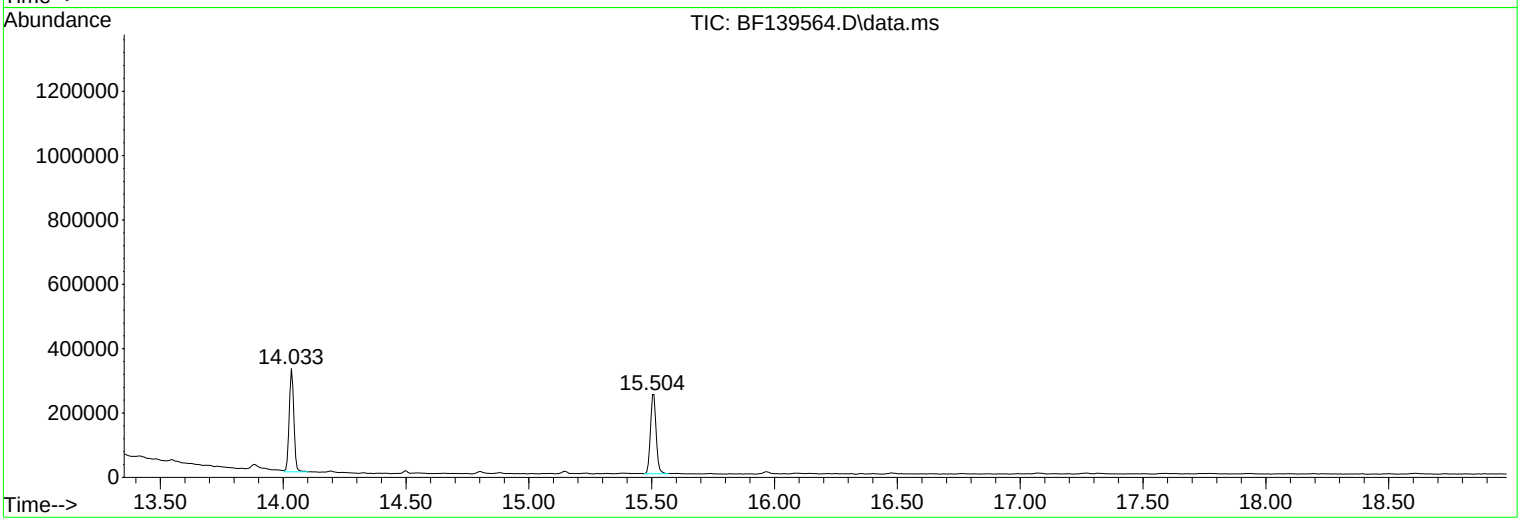
**Instrument :**
BNA_F
**ClientSampleId :**
TP1-5-WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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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Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
BNA_F
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TP1-5-WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

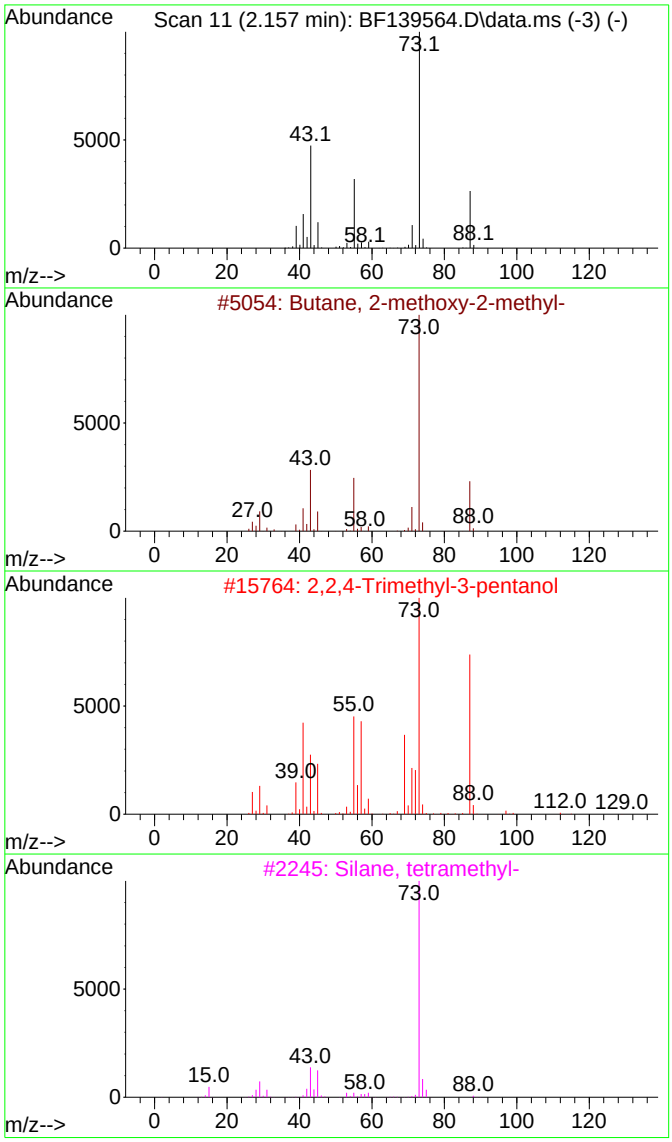
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

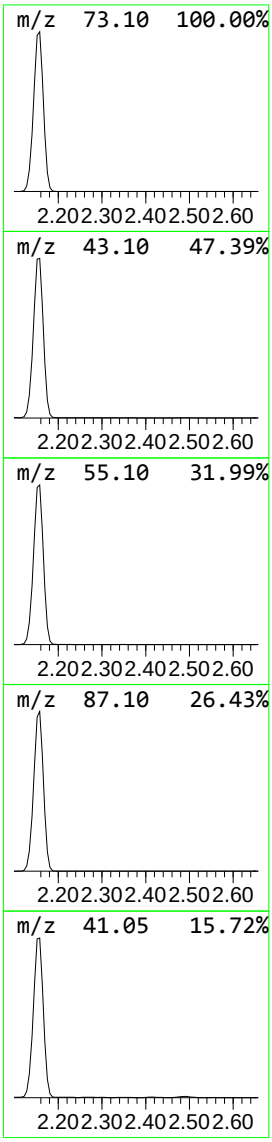
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.157 | 101.24 ng | 2151420 | 1,4-Dichlorobenzene-d4 | 6.875 |

| 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 | Silane, tetramethyl- | 88 | C4H12Si | 000075-76-3 | 38 |
| 4 | 1,3-Dioxolane, 2-methyl- | 88 | C4H8O2 | 000497-26-7 | 23 |
| 5 | Acetamide, N-ethyl- | 87 | C4H9NO | 000625-50-3 | 9 |



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Data File : BF139564.D
Acq On : 26 Sep 2024 23:48
Operator : RC/JU
Sample : P4198-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP1-5-WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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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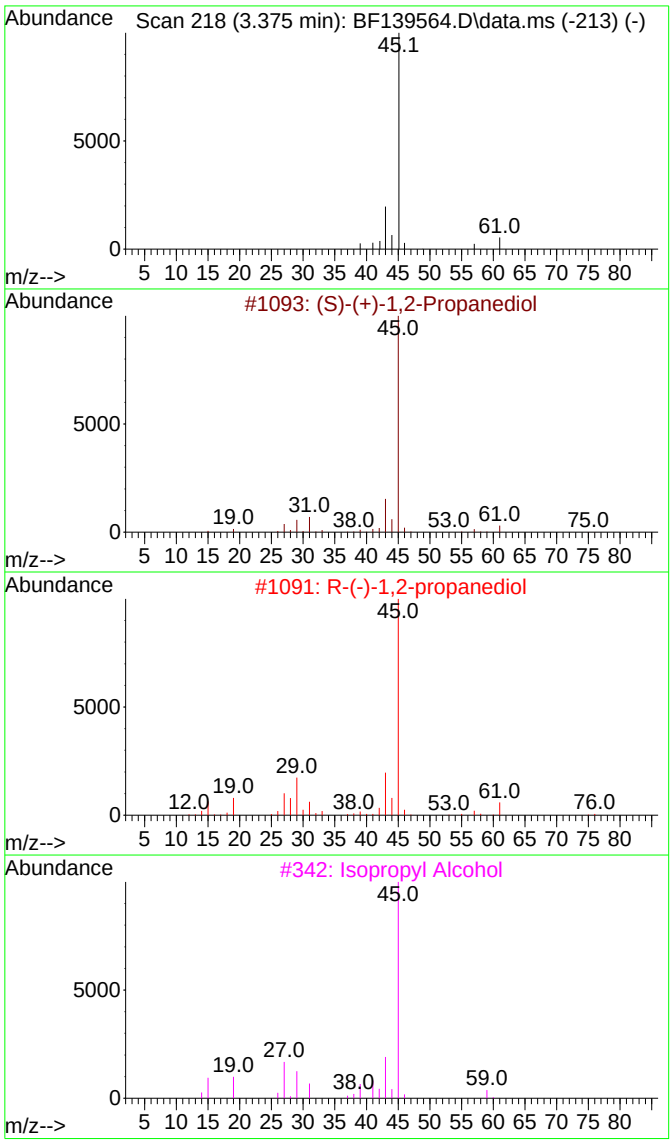
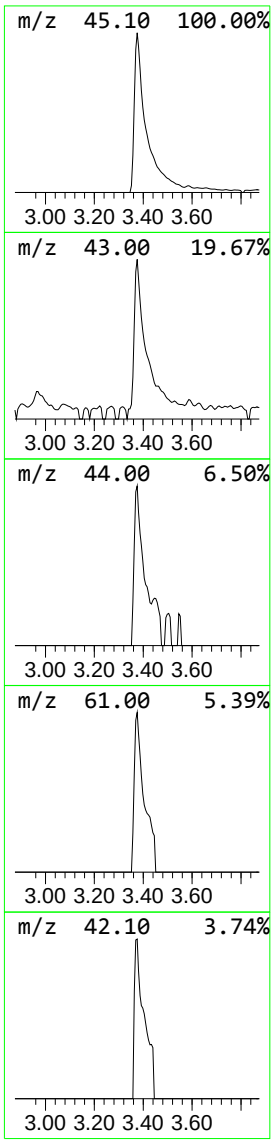
Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 3.375 | 3.01 ng | 63897 | 1,4-Dichlorobenzene-d4 | 6.875 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | (S)-(+)-1,2-Propanediol | 76 | C3H8O2 | 004254-15-3 | 74 |
| 2 | R-(-)-1,2-propanediol | 76 | C3H8O2 | 004254-14-2 | 64 |
| 3 | Isopropyl Alcohol | 60 | C3H8O | 000067-63-0 | 9 |
| 4 | Propylene Glycol | 76 | C3H8O2 | 000057-55-6 | 9 |
| 5 | Formamide | 45 | CH3NO | 000075-12-7 | 5 |



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092624\
Data File : BF139564.D
Acq On : 26 Sep 2024 23:48
Operator : RC/JU
Sample : P4198-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP1-5-WC-1

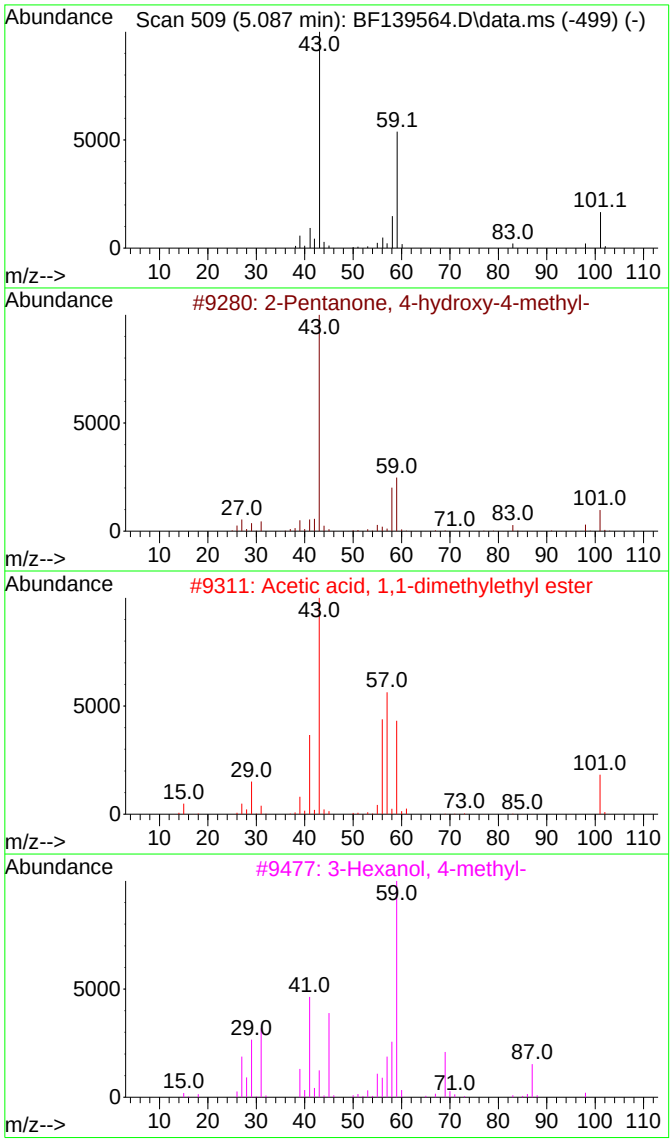
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

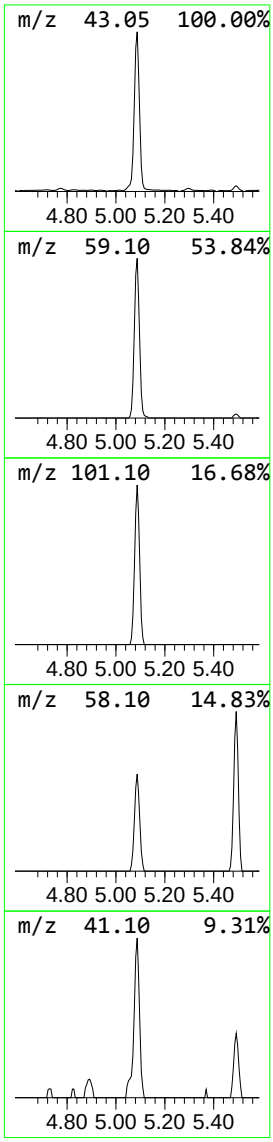
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.087 | 5.24 ng | 111276 | 1,4-Dichlorobenzene-d4 | 6.875 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 59 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 38 |
| 3 | 3-Hexanol, 4-methyl- | 116 | C7H16O | 000615-29-2 | 33 |
| 4 | 2,3-Butanedione, monooxime | 101 | C4H7NO2 | 000057-71-6 | 27 |
| 5 | 1-Propen-2-ol, acetate | 100 | C5H8O2 | 000108-22-5 | 12 |



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Operator : RC/JU
Sample : P4198-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP1-5-WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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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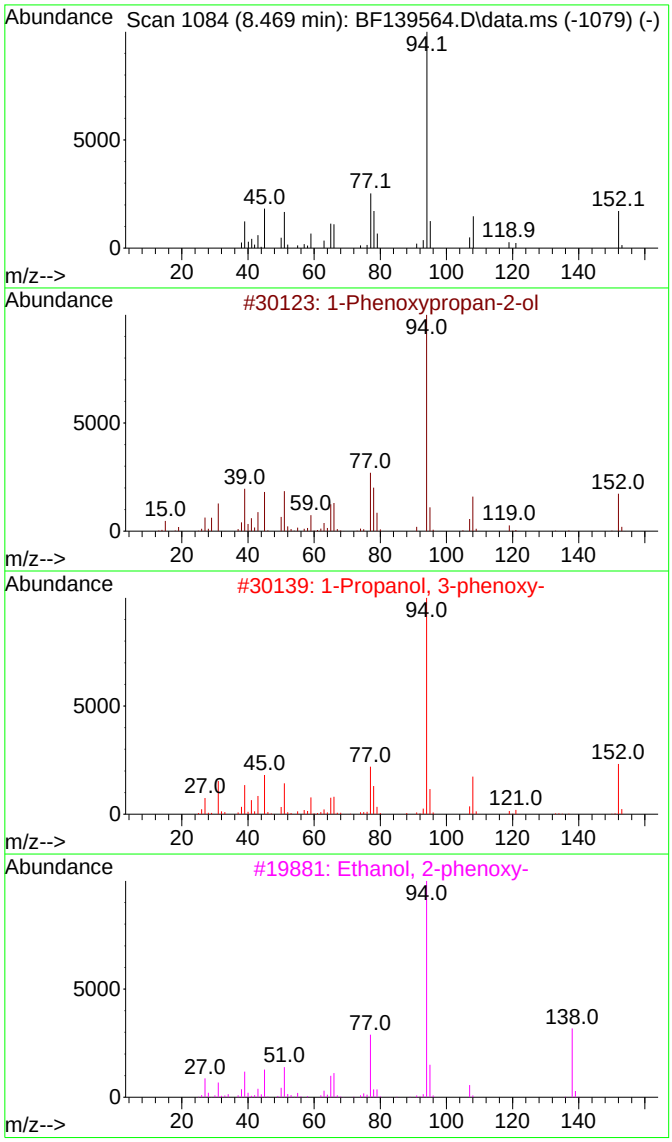
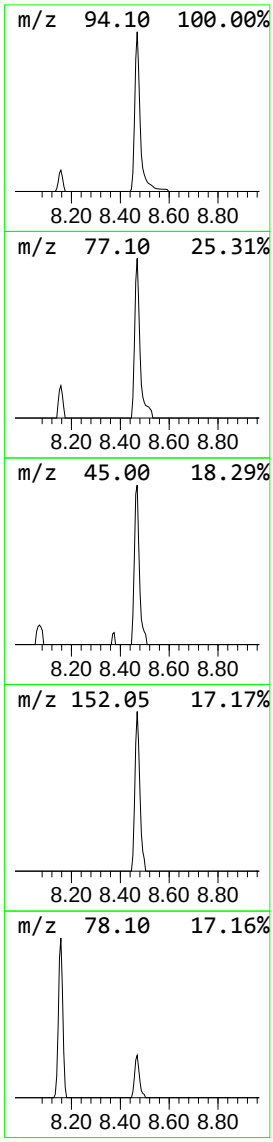
Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.469 | 2.29 ng | 61085 | Naphthalene-d8 | 8.157 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Phenoxypropan-2-ol | 152 | C9H12O2 | 000770-35-4 | 96 |
| 2 | 1-Propanol, 3-phenoxy- | 152 | C9H12O2 | 006180-61-6 | 91 |
| 3 | Ethanol, 2-phenoxy- | 138 | C8H10O2 | 000122-99-6 | 64 |
| 4 | 1-Propanol, 2-phenoxy- | 152 | C9H12O2 | 004169-04-4 | 64 |
| 5 | 3-(.alpha.-Hydroxyethyl)-aniline | 137 | C8H11NO | 002454-37-7 | 59 |



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Acq On : 26 Sep 2024 23:48
Operator : RC/JU
Sample : P4198-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
TP1-5-WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
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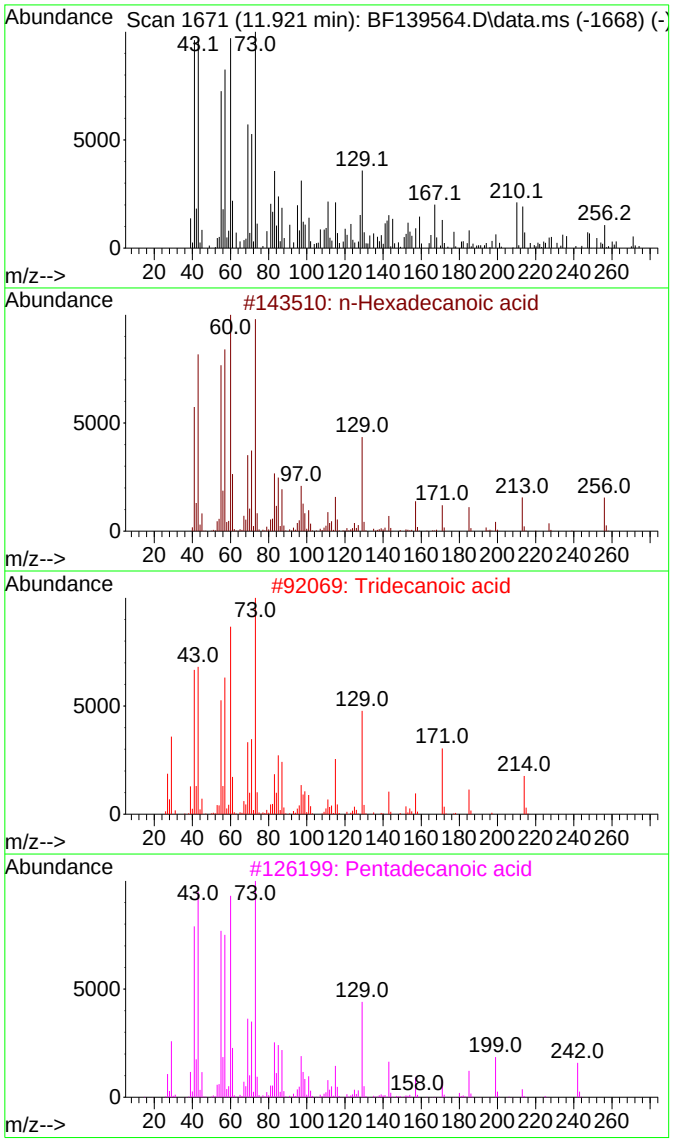
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

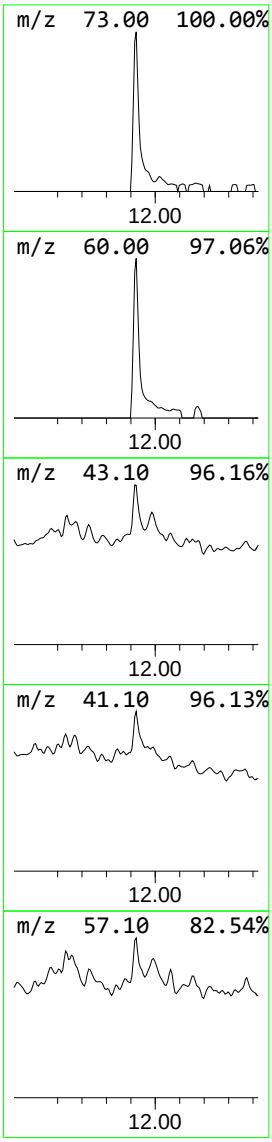
**********

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.922 | 2.34 ng | 71264 | Phenanthrene-d10 | 11.398 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 95 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 95 |
| 3 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 49 |
| 4 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 49 |
| 5 | 2-Methyl-Z-4-tetradecene | 210 | C15H30 | 1000130-78-3 | 38 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092624\
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Misc :
ALS Vial : 19 Sample Multiplier: 1

**Instrument :**
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TP1-5-WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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... | 2.157 | 101.2 | ng | 2151420 | 1 | 6.875 | 425000 | 20.0 |
| (S)-(+)-1,2-Pro... | 3.375 | 3.0 | ng | 63897 | 1 | 6.875 | 425000 | 20.0 |
| 2-Pentanone, 4-... | 5.087 | 5.2 | ng | 111276 | 1 | 6.875 | 425000 | 20.0 |
| 1-Phenoxypropan... | 8.469 | 2.3 | ng | 61085 | 2 | 8.157 | 534393 | 20.0 |
| n-Hexadecanoic ... | 11.922 | 2.3 | ng | 71264 | 4 | 11.398 | 608522 | 20.0 |