

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF071524\  
 Data File : BF138574.D  
 Acq On : 15 Jul 2024 18:14  
 Operator : CG\JU  
 Sample : P3228-01 2X  
 Misc :  
 ALS Vial : 12 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PAT-DIS-01-07112024

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-BF070924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138574.D\data.ms

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 2.134       | 3             | 8           | 14           | rVB      | 822252         | 983163        | 80.68%          | 8.532%        |
| 2         | 3.934       | 309           | 314         | 319          | rBV      | 13925          | 18258         | 1.50%           | 0.158%        |
| 3         | 5.075       | 505           | 508         | 513          | rBV      | 86470          | 87846         | 7.21%           | 0.762%        |
| 4         | 5.487       | 574           | 578         | 589          | rBV      | 1417212        | 1218620       | 100.00%         | 10.575%       |
| 5         | 6.498       | 746           | 750         | 753          | rBV      | 1481086        | 1214035       | 99.62%          | 10.536%       |
| 6         | 6.863       | 809           | 812         | 816          | rVB      | 747636         | 594457        | 48.78%          | 5.159%        |
| 7         | 7.428       | 903           | 908         | 911          | rBV      | 889115         | 787900        | 64.66%          | 6.838%        |
| 8         | 7.680       | 946           | 951         | 955          | rVB2     | 25533          | 28247         | 2.32%           | 0.245%        |
| 9         | 8.145       | 1024          | 1030        | 1033         | rBV      | 944752         | 735167        | 60.33%          | 6.380%        |
| 10        | 8.457       | 1081          | 1083        | 1086         | rBV      | 24845          | 24506         | 2.01%           | 0.213%        |
| 11        | 9.163       | 1200          | 1203        | 1205         | rBV2     | 18341          | 16509         | 1.35%           | 0.143%        |
| 12        | 9.222       | 1209          | 1213        | 1216         | rVV      | 1392015        | 1203773       | 98.78%          | 10.447%       |
| 13        | 9.257       | 1216          | 1219        | 1222         | rVV5     | 23706          | 29632         | 2.43%           | 0.257%        |
| 14        | 9.292       | 1222          | 1225        | 1229         | rVB3     | 38379          | 39180         | 3.22%           | 0.340%        |
| 15        | 9.369       | 1235          | 1238        | 1240         | rVB3     | 24602          | 21660         | 1.78%           | 0.188%        |
| 16        | 9.533       | 1263          | 1266        | 1268         | rBV4     | 17760          | 14867         | 1.22%           | 0.129%        |
| 17        | 9.604       | 1276          | 1278        | 1282         | rBV4     | 31645          | 43169         | 3.54%           | 0.375%        |
| 18        | 9.645       | 1282          | 1285        | 1289         | rBV3     | 24283          | 31438         | 2.58%           | 0.273%        |
| 19        | 9.763       | 1302          | 1305        | 1308         | rBV4     | 28645          | 38065         | 3.12%           | 0.330%        |
| 20        | 9.810       | 1310          | 1313        | 1315         | rVB3     | 31319          | 29953         | 2.46%           | 0.260%        |
| 21        | 9.898       | 1325          | 1328        | 1332         | rBV      | 801091         | 617943        | 50.71%          | 5.363%        |
| 22        | 9.998       | 1341          | 1345        | 1350         | rVB4     | 37854          | 50958         | 4.18%           | 0.442%        |
| 23        | 10.210      | 1379          | 1381        | 1383         | rBV2     | 22413          | 23836         | 1.96%           | 0.207%        |
| 24        | 10.233      | 1383          | 1385        | 1389         | rVB5     | 27956          | 33520         | 2.75%           | 0.291%        |
| 25        | 10.304      | 1394          | 1397        | 1399         | rBV4     | 19642          | 20458         | 1.68%           | 0.178%        |
| 26        | 10.686      | 1458          | 1462        | 1467         | rBV      | 645038         | 546560        | 44.85%          | 4.743%        |
| 27        | 10.810      | 1480          | 1483        | 1490         | rVB      | 40570          | 46882         | 3.85%           | 0.407%        |
| 28        | 11.021      | 1516          | 1519        | 1521         | rBV4     | 14760          | 16221         | 1.33%           | 0.141%        |
| 29        | 11.186      | 1545          | 1547        | 1552         | rVB5     | 14772          | 14978         | 1.23%           | 0.130%        |
| 30        | 11.274      | 1560          | 1562        | 1567         | rVB4     | 37088          | 48654         | 3.99%           | 0.422%        |
| 31        | 11.386      | 1577          | 1581        | 1583         | rBV      | 644694         | 564680        | 46.34%          | 4.900%        |
| 32        | 11.410      | 1583          | 1585        | 1591         | rVB      | 110292         | 93371         | 7.66%           | 0.810%        |
| 33        | 11.457      | 1591          | 1593        | 1596         | rBV      | 20047          | 18123         | 1.49%           | 0.157%        |
| 34        | 11.910      | 1667          | 1670        | 1674         | rVB2     | 72204          | 82900         | 6.80%           | 0.719%        |
| 35        | 11.998      | 1682          | 1685        | 1687         | rBV3     | 24583          | 23931         | 1.96%           | 0.208%        |
| 36        | 12.180      | 1714          | 1716        | 1718         | rBV      | 18275          | 15210         | 1.25%           | 0.132%        |

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Operator : CG\JU  
Sample : P3228-01 2X  
Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PAT-DIS-01-07112024

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-BF070924.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |         |        |        |        |
|----|--------|------|------|------|------|---------|--------|--------|--------|
| 37 | 12.433 | 1757 | 1759 | 1762 | rBV2 | 24482   | 19704  | 1.62%  | 0.171% |
| 38 | 12.598 | 1784 | 1787 | 1791 | rBV  | 163859  | 142115 | 11.66% | 1.233% |
| 39 | 12.692 | 1800 | 1803 | 1807 | rBV5 | 41359   | 46922  | 3.85%  | 0.407% |
| 40 | 12.827 | 1823 | 1826 | 1833 | rVB  | 154422  | 145844 | 11.97% | 1.266% |
| 41 | 12.968 | 1846 | 1850 | 1853 | rBV  | 1097935 | 933020 | 76.56% | 8.097% |
| 42 | 14.021 | 2025 | 2029 | 2032 | rBV  | 480871  | 474287 | 38.92% | 4.116% |
| 43 | 15.492 | 2276 | 2279 | 2287 | rVB  | 270710  | 382519 | 31.39% | 3.320% |

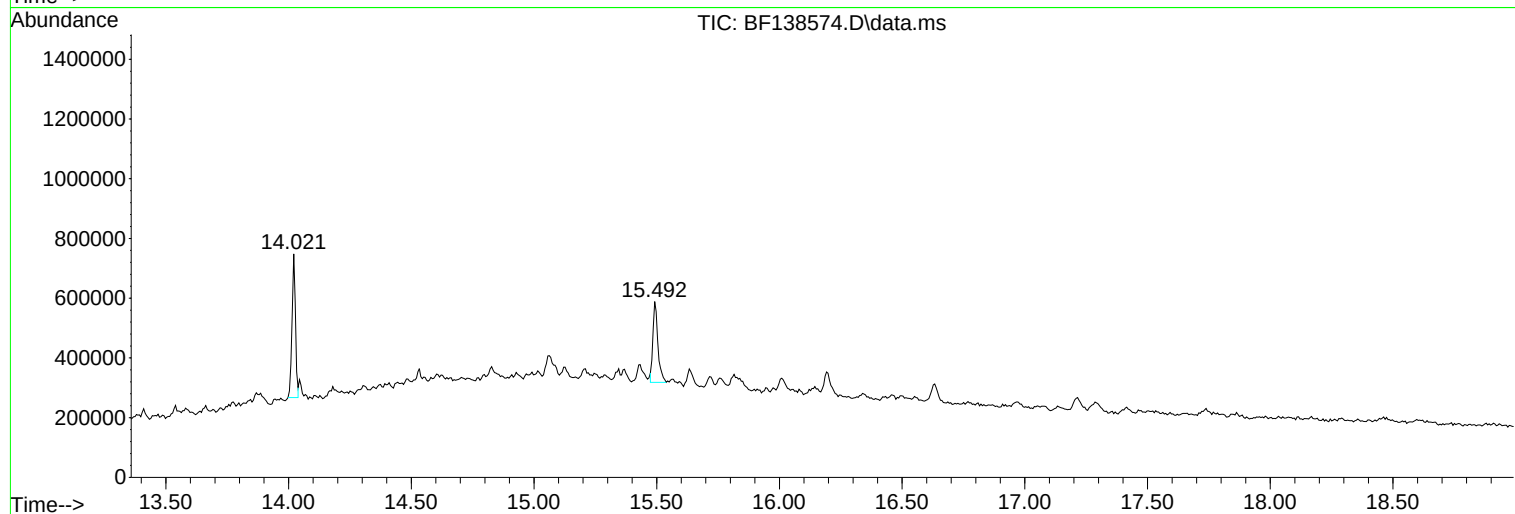
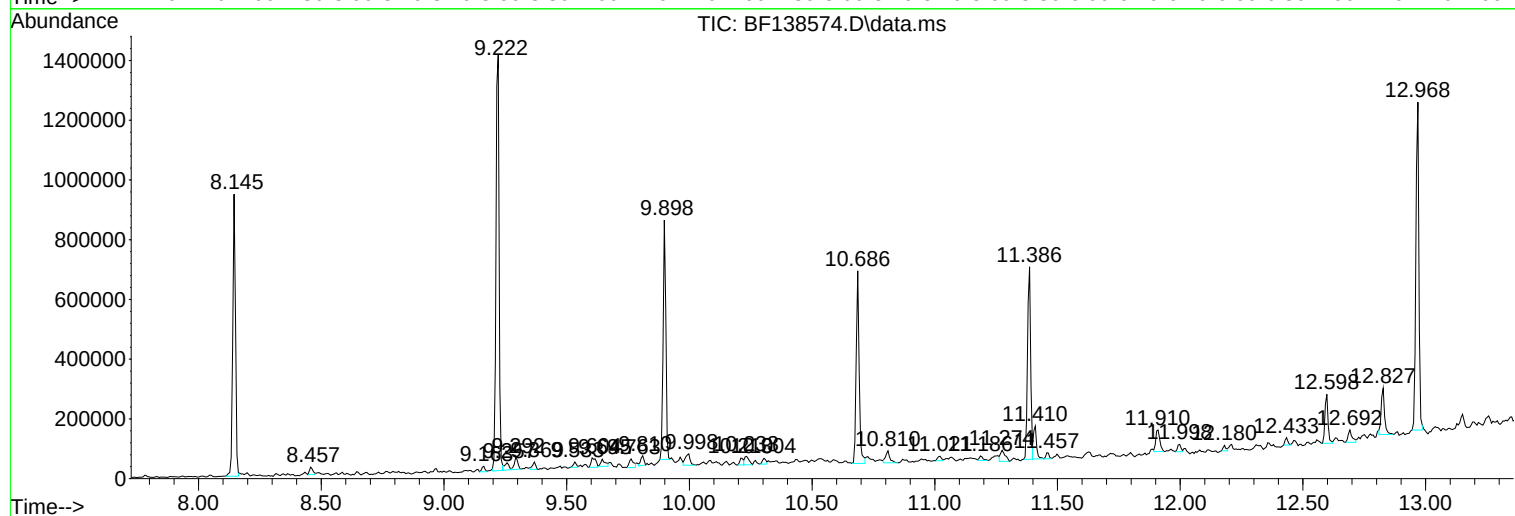
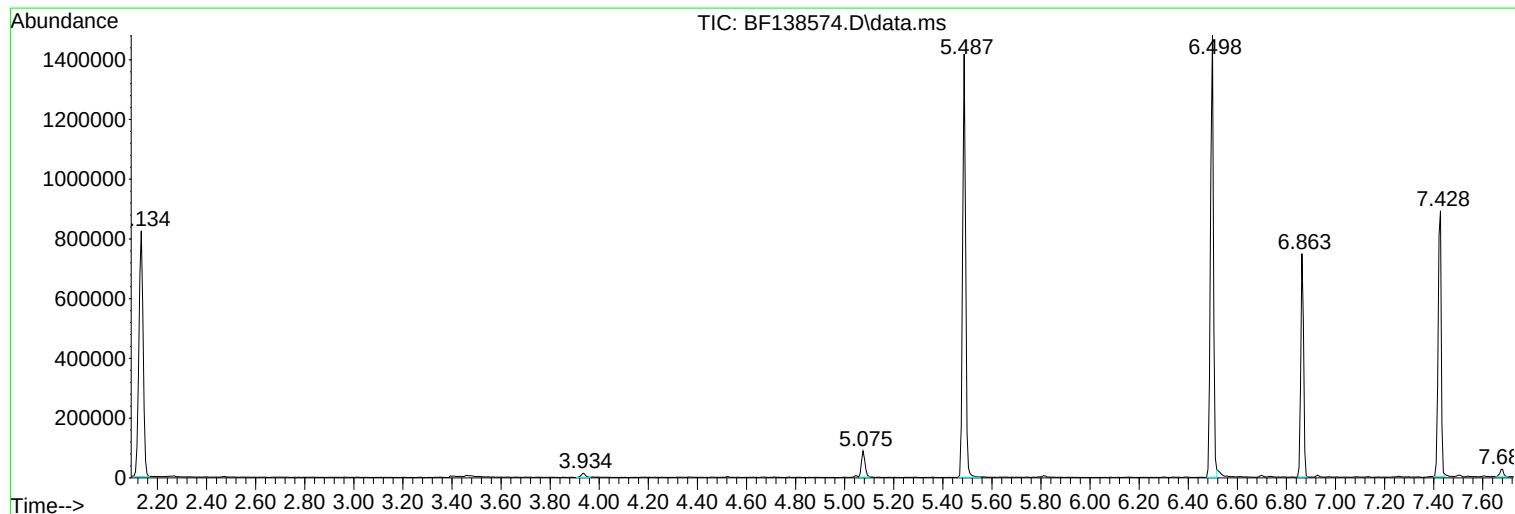
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Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PAT-DIS-01-07112024

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF070924.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\BF071524\  
Data File : BF138574.D  
Acq On : 15 Jul 2024 18:14  
Operator : CG\JU  
Sample : P3228-01 2X  
Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PAT-DIS-01-07112024

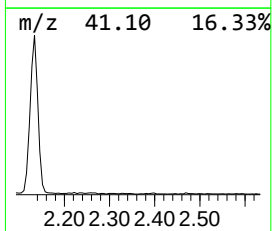
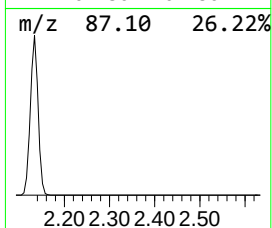
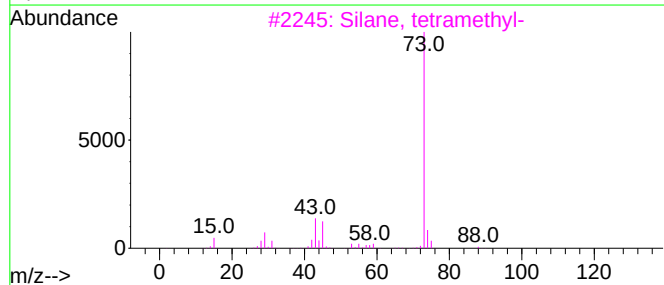
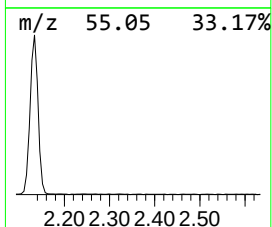
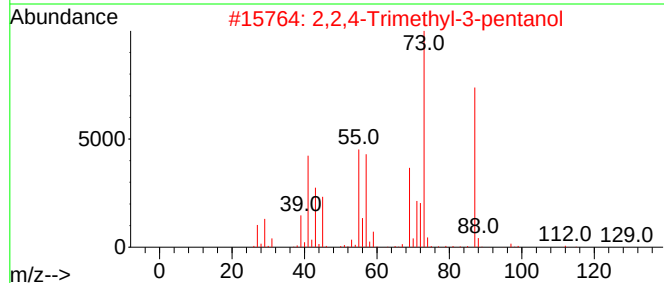
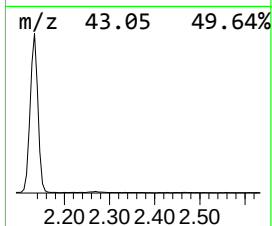
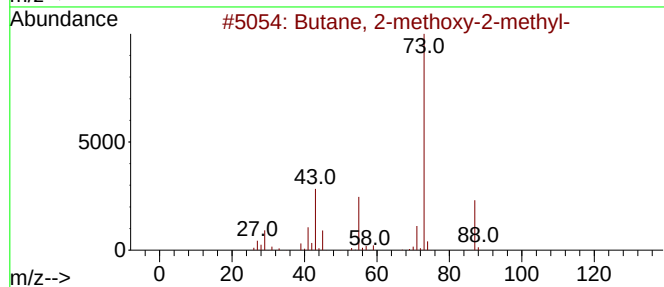
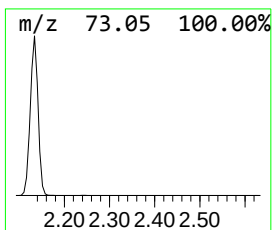
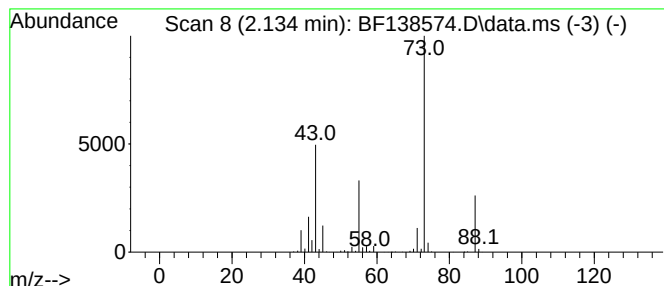
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF070924.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 2.134 | 33.08 ng | 983163 | 1,4-Dichlorobenzene-d4 | 6.863 |

| 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 | 32   |
| 4    |    |   | 1,3-Dioxolane, 2-methyl-    | 88  | C4H8O2  | 000497-26-7 | 23   |
| 5    |    |   | 1,3-Dioxolane, 2-propyl-    | 116 | C6H12O2 | 003390-13-4 | 23   |



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Instrument :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF070924.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

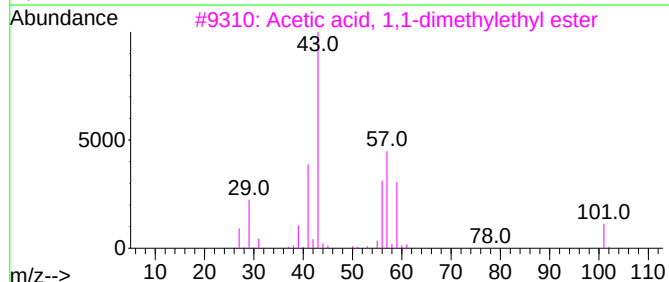
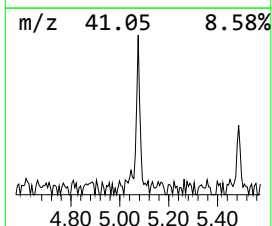
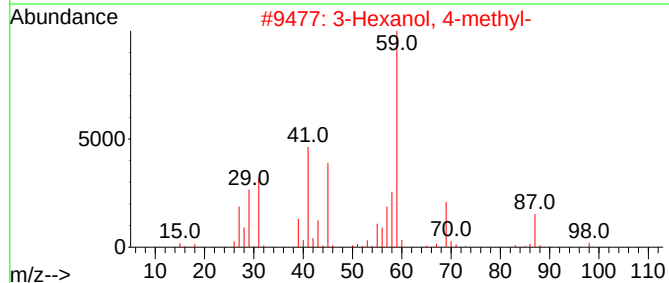
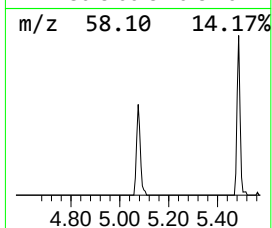
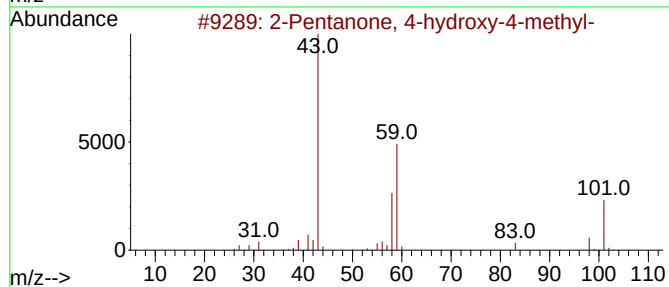
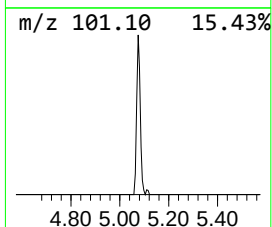
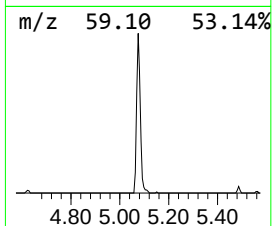
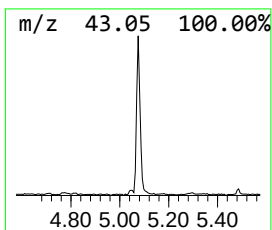
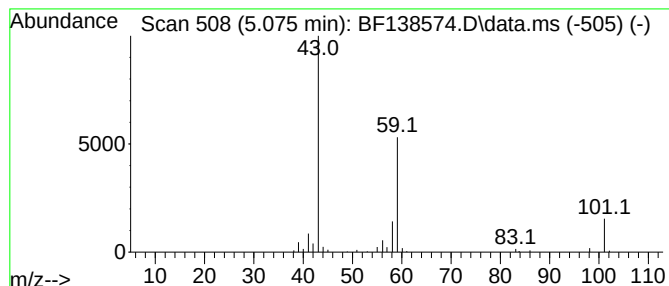
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 5.075 | 2.96 ng | 87846 | 1,4-Dichlorobenzene-d4 | 6.863 |

| Hit# | of 5                                | Tentative ID | MW       | MolForm     | CAS# | Qual |
|------|-------------------------------------|--------------|----------|-------------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-    | 116          | C6H12O2  | 000123-42-2 | 56   |      |
| 2    | 3-Hexanol, 4-methyl-                | 116          | C7H16O   | 000615-29-2 | 40   |      |
| 3    | Acetic acid, 1,1-dimethylethyl e... | 116          | C6H12O2  | 000540-88-5 | 38   |      |
| 4    | 2-Hexanol, 2-methyl-                | 116          | C7H16O   | 000625-23-0 | 28   |      |
| 5    | Acetic acid, cyano-, 1,1-dimethy... | 141          | C7H11NO2 | 001116-98-9 | 25   |      |



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Instrument :  
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PAT-DIS-01-07112024

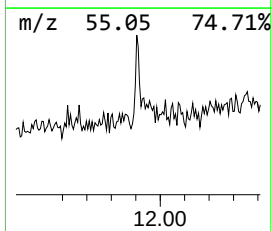
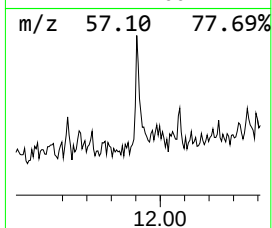
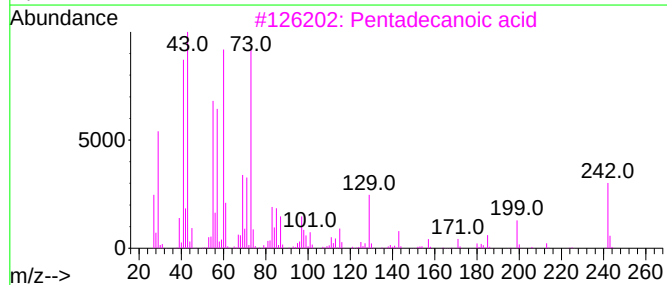
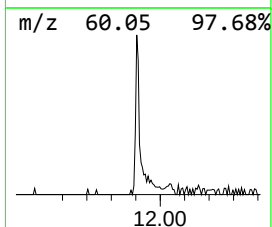
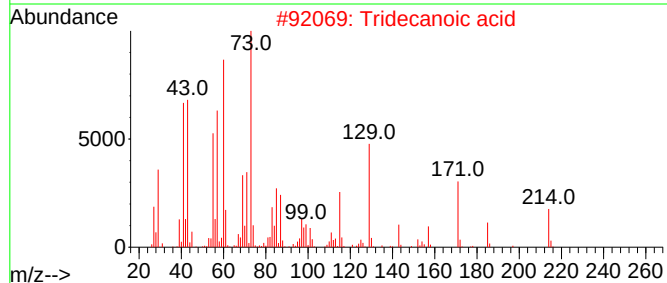
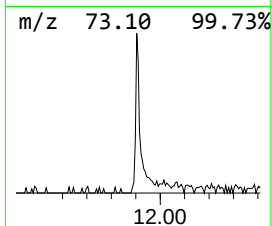
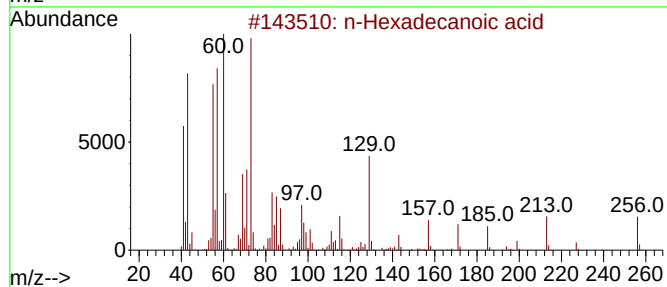
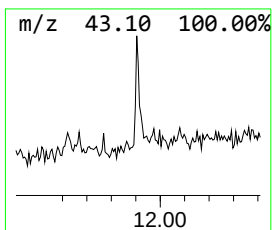
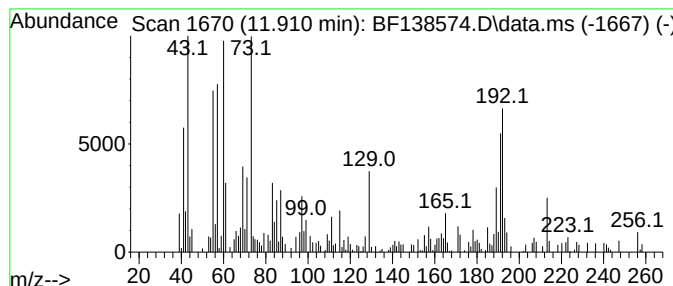
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF070924.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 11.910 | 2.94 ng | 82900 | Phenanthrene-d10 | 11.386 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 90   |
| 2    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 83   |
| 3    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 50   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 46   |
| 5    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 42   |



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Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF070924.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Butane, 2-metho... | 2.134  | 33.1    | ng    | 983163   | 1                     | 6.863  | 594457 | 20.0 |
| 2-Pentanone, 4-... | 5.075  | 3.0     | ng    | 87846    | 1                     | 6.863  | 594457 | 20.0 |
| n-Hexadecanoic ... | 11.910 | 2.9     | ng    | 82900    | 4                     | 11.386 | 564680 | 20.0 |