

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF030223\  
 Data File : BF132615.D  
 Acq On : 02 Mar 2023 19:14  
 Operator : CG\JU  
 Sample : 01749-07  
 Misc :  
 ALS Vial : 12 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 CF-9

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-BF022223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132615.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         | 5.240       | 445           | 451         | 460          | rVB      | 1847051        | 2485742       | 46.55%          | 6.546%        |
| 2         | 5.628       | 512           | 517         | 521          | rBV      | 4437646        | 4901745       | 91.80%          | 12.909%       |
| 3         | 6.628       | 682           | 687         | 690          | rBV      | 4460615        | 5065858       | 94.88%          | 13.341%       |
| 4         | 6.698       | 696           | 699         | 702          | rBV      | 244534         | 190843        | 3.57%           | 0.503%        |
| 5         | 6.728       | 702           | 704         | 708          | rBV3     | 48443          | 59303         | 1.11%           | 0.156%        |
| 6         | 6.998       | 747           | 750         | 754          | rBV      | 1466638        | 1207611       | 22.62%          | 3.180%        |
| 7         | 7.069       | 760           | 762         | 766          | rVB      | 180091         | 143336        | 2.68%           | 0.377%        |
| 8         | 7.110       | 766           | 769         | 772          | rBV      | 212408         | 162731        | 3.05%           | 0.429%        |
| 9         | 7.569       | 842           | 847         | 850          | rBV      | 3466096        | 3342778       | 62.61%          | 8.803%        |
| 10        | 8.286       | 965           | 969         | 971          | rBV      | 1962300        | 1548142       | 28.99%          | 4.077%        |
| 11        | 8.304       | 971           | 972         | 976          | rVB      | 179837         | 140238        | 2.63%           | 0.369%        |
| 12        | 9.363       | 1148          | 1152        | 1155         | rBV      | 5896538        | 5339415       | 100.00%         | 14.061%       |
| 13        | 10.045      | 1265          | 1268        | 1272         | rBV      | 1866931        | 1582663       | 29.64%          | 4.168%        |
| 14        | 10.763      | 1386          | 1390        | 1393         | rVB      | 150916         | 128816        | 2.41%           | 0.339%        |
| 15        | 10.839      | 1399          | 1403        | 1407         | rBV      | 3101809        | 2892669       | 54.18%          | 7.618%        |
| 16        | 11.545      | 1519          | 1523        | 1526         | rBV      | 1436949        | 1316383       | 24.65%          | 3.467%        |
| 17        | 11.945      | 1588          | 1591        | 1595         | rVB      | 112649         | 91015         | 1.70%           | 0.240%        |
| 18        | 12.057      | 1607          | 1610        | 1624         | rBV2     | 246521         | 407528        | 7.63%           | 1.073%        |
| 19        | 12.586      | 1697          | 1700        | 1703         | rBV      | 111050         | 99319         | 1.86%           | 0.262%        |
| 20        | 12.763      | 1727          | 1730        | 1733         | rBV      | 73344          | 70563         | 1.32%           | 0.186%        |
| 21        | 12.798      | 1733          | 1736        | 1738         | rVV      | 87268          | 73079         | 1.37%           | 0.192%        |
| 22        | 12.827      | 1738          | 1741        | 1743         | rVV      | 99082          | 90175         | 1.69%           | 0.237%        |
| 23        | 12.851      | 1743          | 1745        | 1757         | rVB2     | 71721          | 104589        | 1.96%           | 0.275%        |
| 24        | 13.133      | 1789          | 1793        | 1797         | rBV      | 3786932        | 3828159       | 71.70%          | 10.081%       |
| 25        | 14.045      | 1942          | 1948        | 1964         | rBV3     | 167972         | 551239        | 10.32%          | 1.452%        |
| 26        | 14.162      | 1965          | 1968        | 1971         | rBV      | 122106         | 95036         | 1.78%           | 0.250%        |
| 27        | 14.204      | 1971          | 1975        | 1978         | rBV      | 1231987        | 1083483       | 20.29%          | 2.853%        |
| 28        | 15.756      | 2234          | 2239        | 2247         | rVB      | 753951         | 969772        | 18.16%          | 2.554%        |

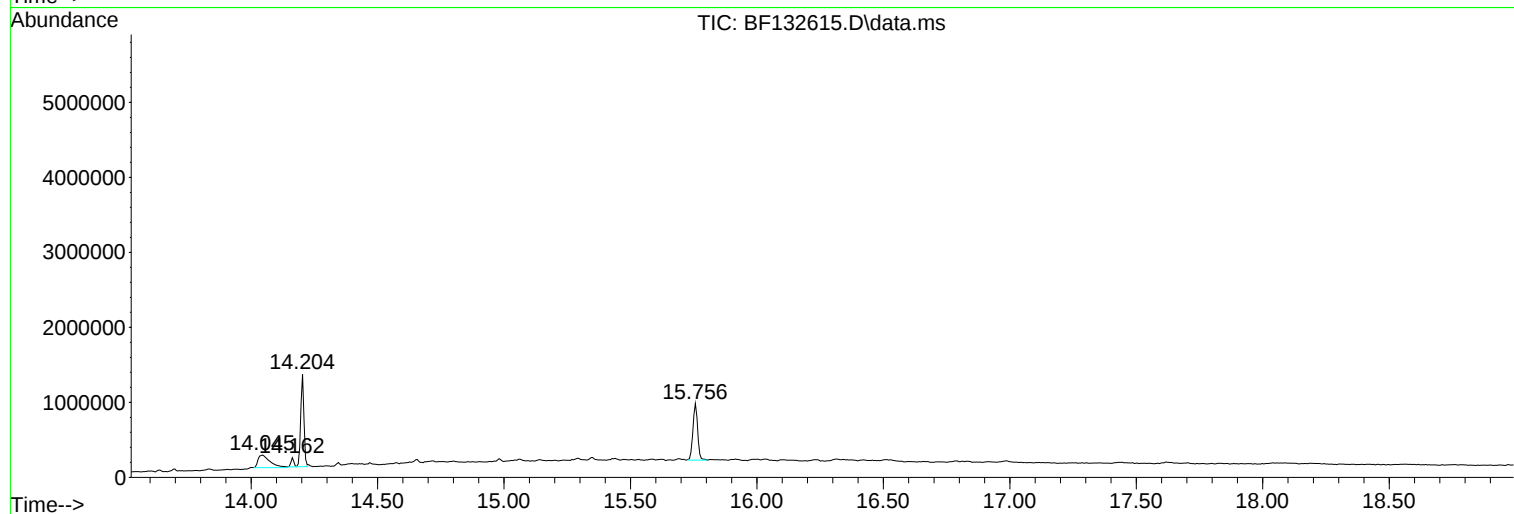
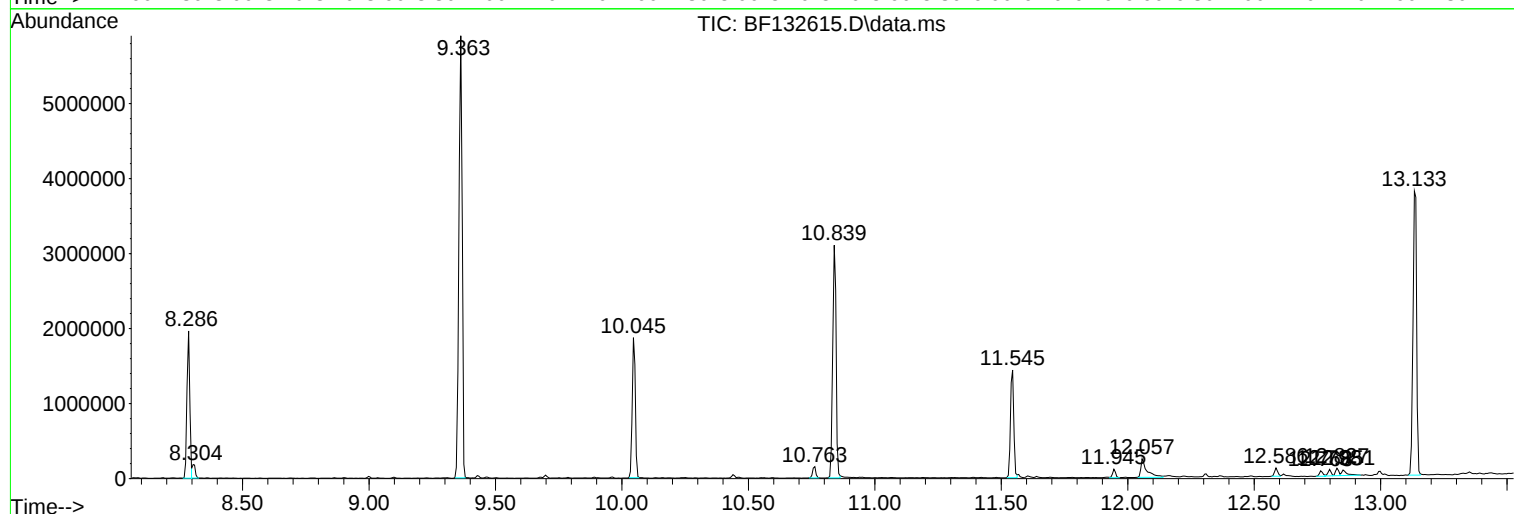
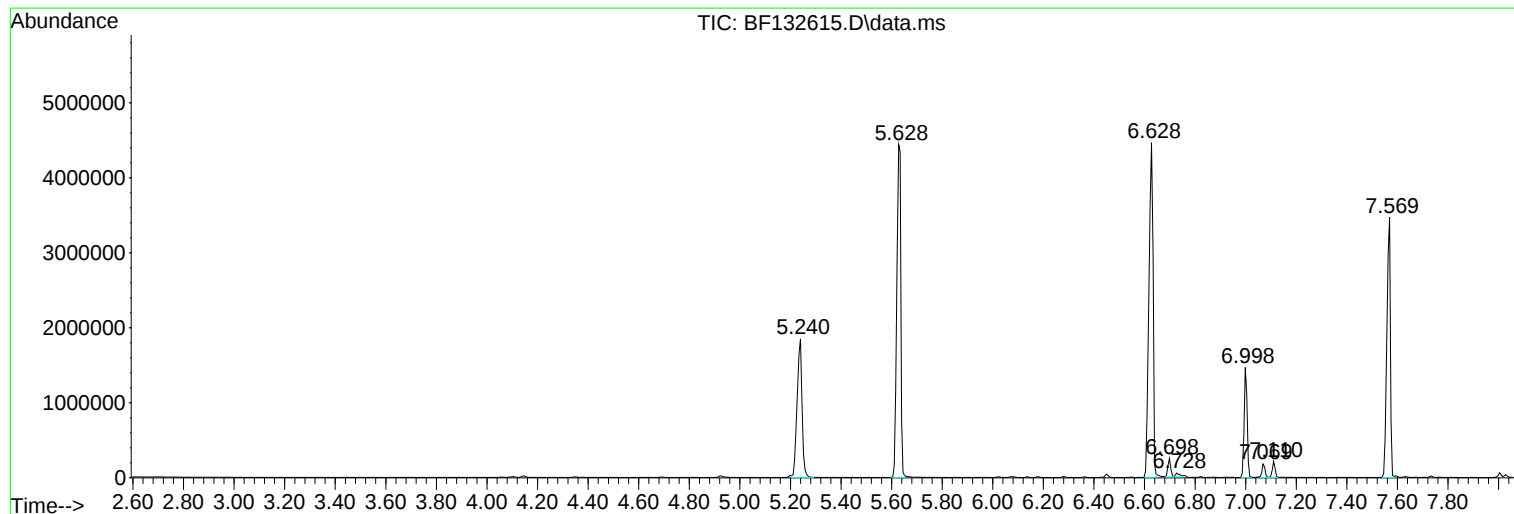
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ALS Vial : 12 Sample Multiplier: 1

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BNA\_F  
ClientSampleId :  
CF-9

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF022223.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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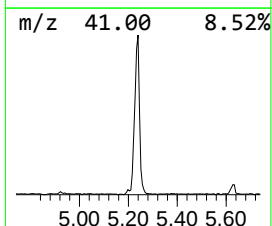
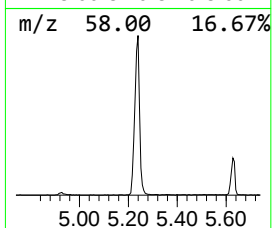
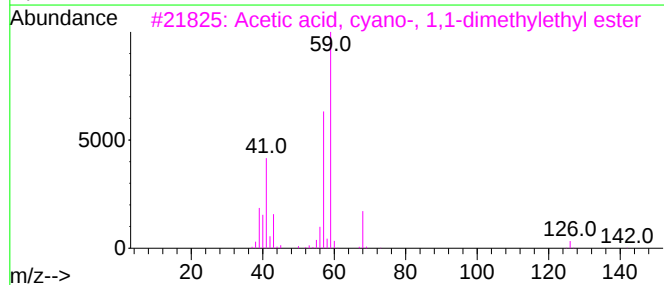
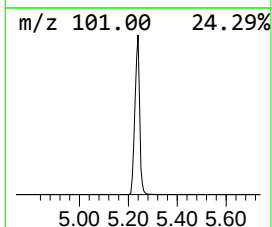
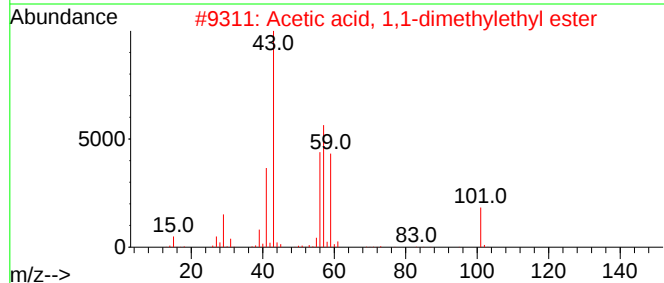
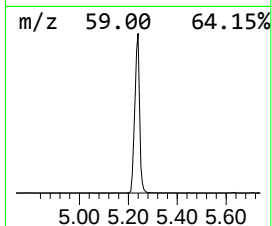
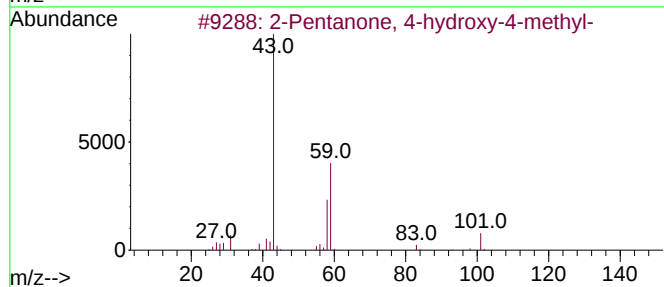
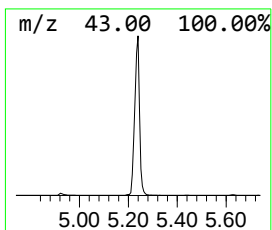
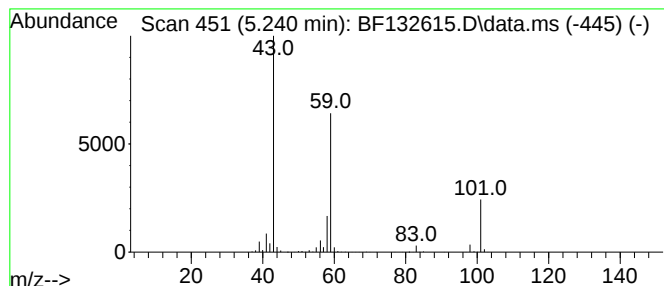
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.  | EstConc  | Area    | Relative to ISTD       | R.T.  |
|-------|----------|---------|------------------------|-------|
| 5.240 | 41.17 ng | 2485740 | 1,4-Dichlorobenzene-d4 | 6.998 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 56   |
| 2    |    |   | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2  | 000540-88-5 | 39   |
| 3    |    |   | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 17   |
| 4    |    |   | 1-Propen-2-ol, acetate              | 100 | C5H8O2   | 000108-22-5 | 10   |
| 5    |    |   | (+)-4-Amino-4,5-dihydro-2(3H)-f...  | 101 | C4H7NO2  | 016504-58-8 | 9    |



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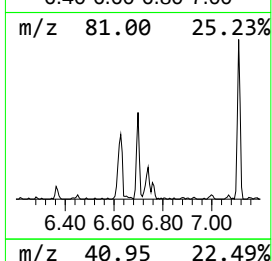
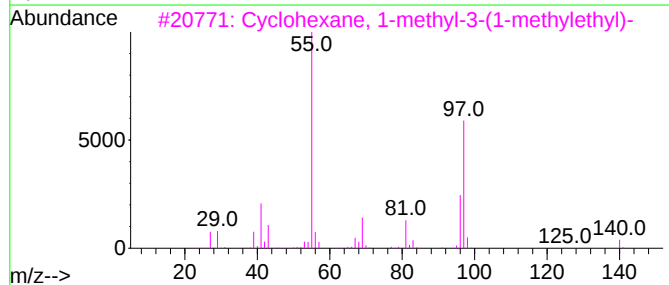
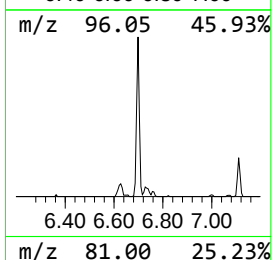
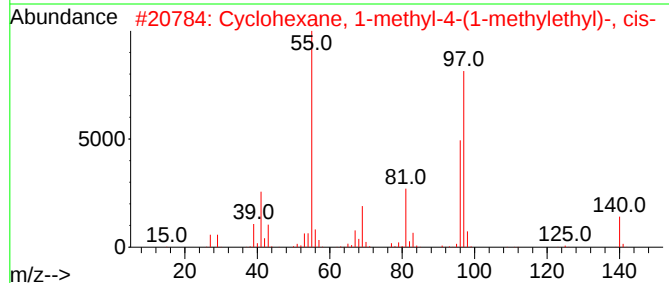
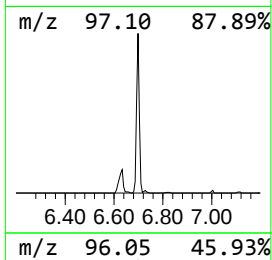
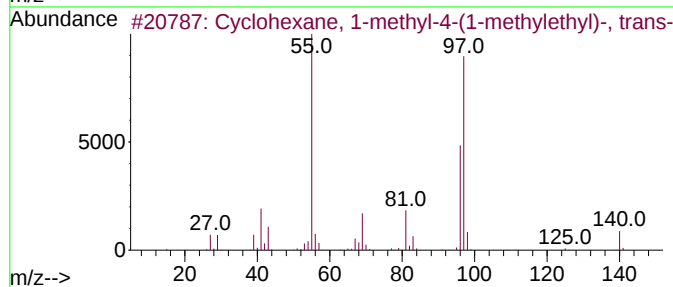
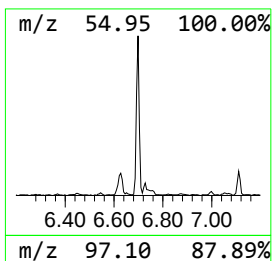
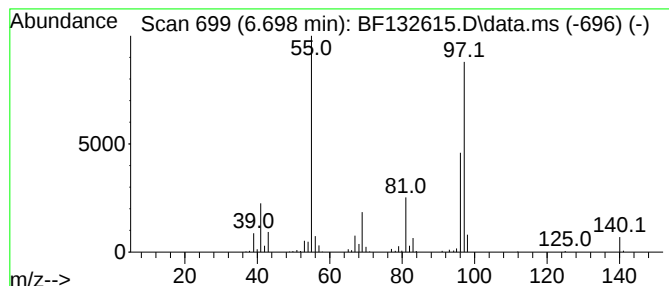
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF022223.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Cyclohexane, 1-methyl-4-(1-... Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 6.698 | 3.16 ng | 190843 | 1,4-Dichlorobenzene-d4 | 6.998 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Cyclohexane, 1-methyl-4-(1-methy... | 140 | C10H20  | 001678-82-6 | 94   |
| 2    |    |   | Cyclohexane, 1-methyl-4-(1-methy... | 140 | C10H20  | 006069-98-3 | 94   |
| 3    |    |   | Cyclohexane, 1-methyl-3-(1-methy... | 140 | C10H20  | 016580-24-8 | 91   |
| 4    |    |   | 1-Methyl-4-(1-methylethyl)-cyclo... | 140 | C10H20  | 000099-82-1 | 91   |
| 5    |    |   | m-Menthane, (1S,3S)-(+)-            | 140 | C10H20  | 013837-67-7 | 90   |



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Sample : 01749-07  
Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
CF-9

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF022223.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

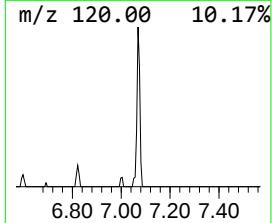
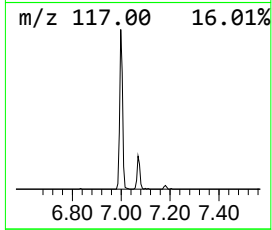
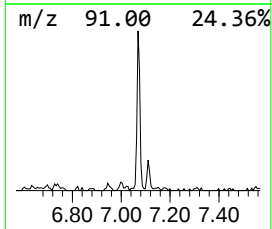
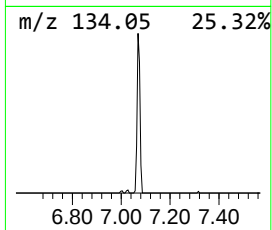
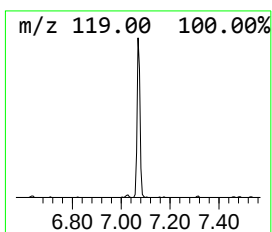
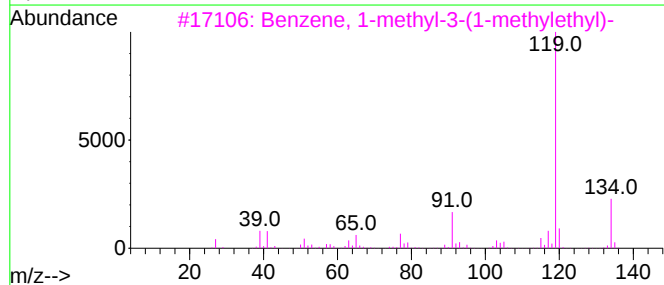
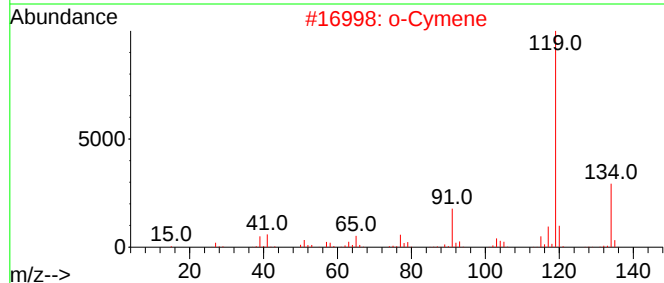
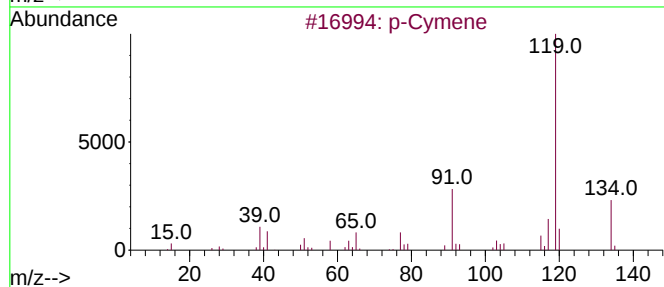
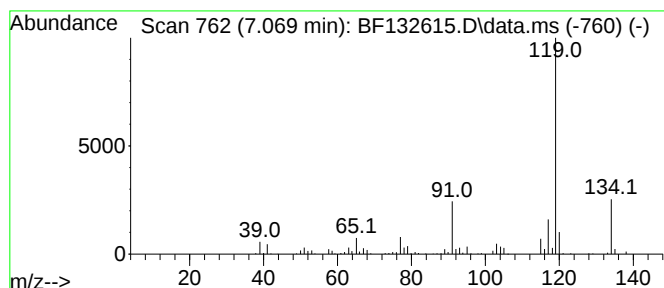
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 p-Cymene Concentration Rank 6

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 7.069 | 2.37 ng | 143336 | 1,4-Dichlorobenzene-d4 | 6.998 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | p-Cymene                            | 134 | C10H14  | 000099-87-6 | 95   |
| 2    |    |   | o-Cymene                            | 134 | C10H14  | 000527-84-4 | 95   |
| 3    |    |   | Benzene, 1-methyl-3-(1-methyleth... | 134 | C10H14  | 000535-77-3 | 91   |
| 4    |    |   | 1,3,5-Cycloheptatriene, 3,7,7-tr... | 134 | C10H14  | 003479-89-8 | 91   |
| 5    |    |   | Benzene, 1,2,3,4-tetramethyl-       | 134 | C10H14  | 000488-23-3 | 90   |



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CF-9

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF022223.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

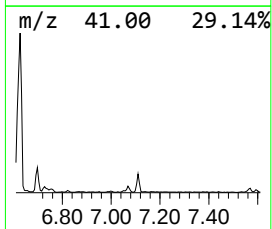
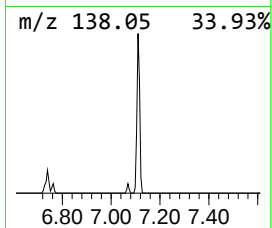
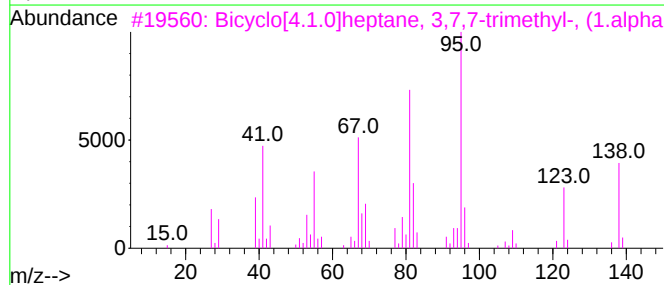
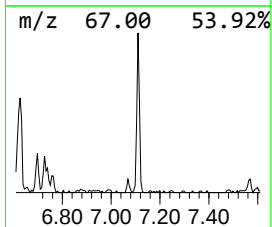
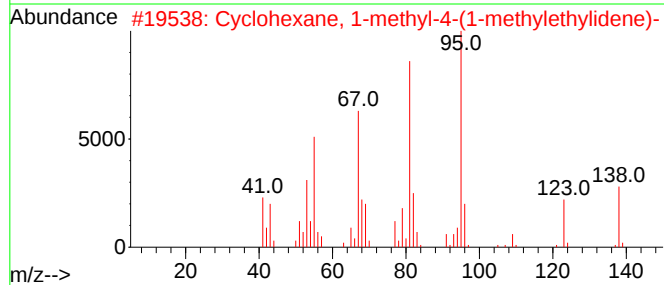
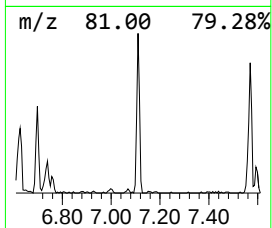
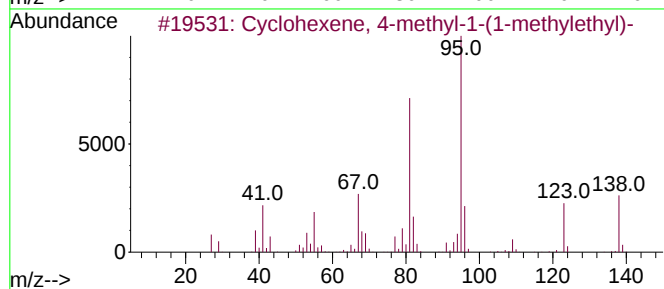
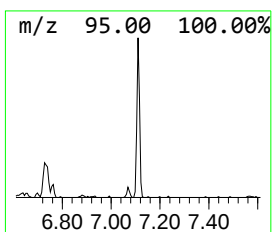
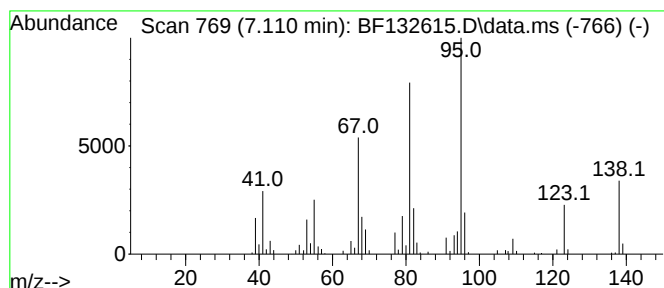
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Cyclohexene, 4-methyl-1-(1-... Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 7.110 | 2.70 ng | 162731 | 1,4-Dichlorobenzene-d4 | 6.998 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Cyclohexene, 4-methyl-1-(1-methy... | 138 | C10H18  | 000500-00-5 | 96   |
| 2    |    |   | Cyclohexane, 1-methyl-4-(1-methy... | 138 | C10H18  | 001124-27-2 | 96   |
| 3    |    |   | Bicyclo[4.1.0]heptane, 3,7,7-tri... | 138 | C10H18  | 018968-23-5 | 87   |
| 4    |    |   | Cyclohexene, 4-methyl-1-(1-methy... | 138 | C10H18  | 000619-52-3 | 87   |
| 5    |    |   | Bicyclo[4.1.0]heptane, 3,7,7-tri... | 138 | C10H18  | 002778-68-9 | 86   |



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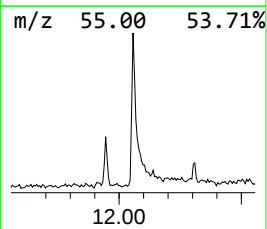
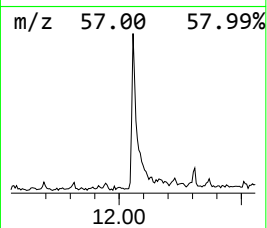
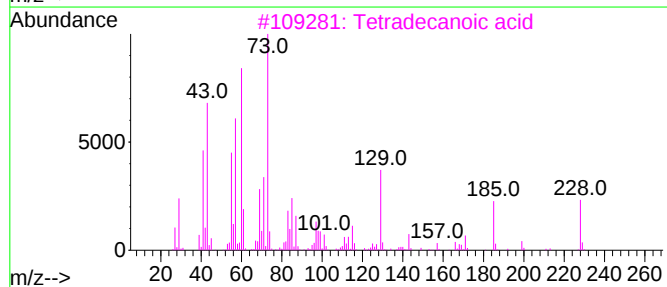
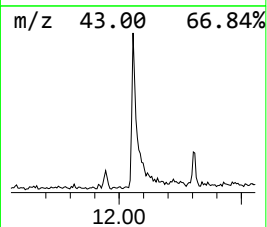
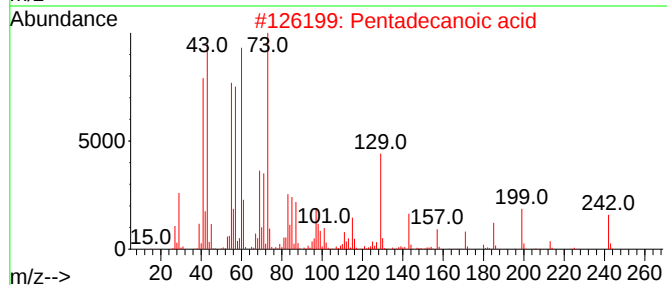
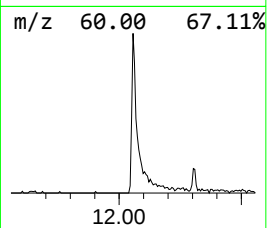
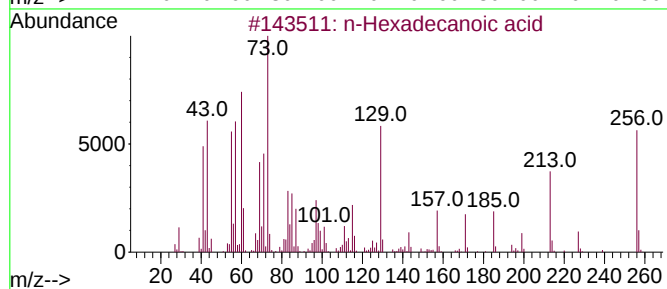
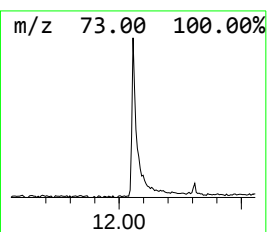
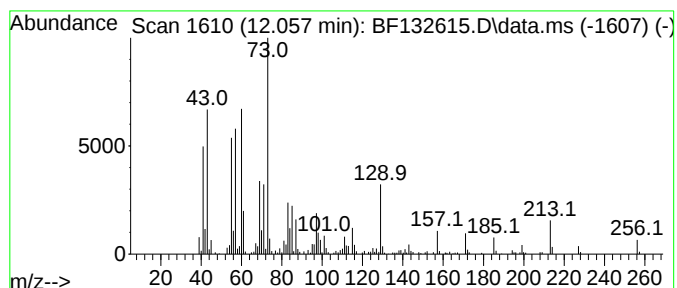
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 12.057 | 6.19 ng | 407528 | Phenanthrene-d10 | 11.545 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 81   |
| 3    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 72   |
| 4    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 64   |
| 5    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 38   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF030223\  
Data File : BF132615.D  
Acq On : 02 Mar 2023 19:14  
Operator : CG\JU  
Sample : 01749-07  
Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
CF-9

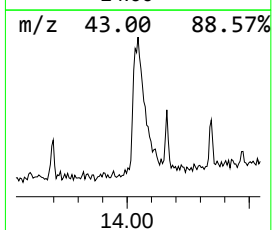
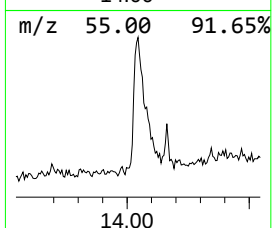
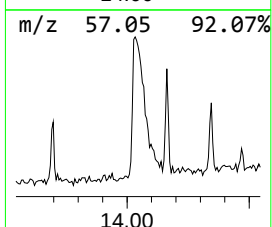
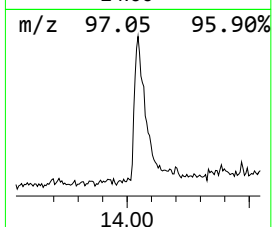
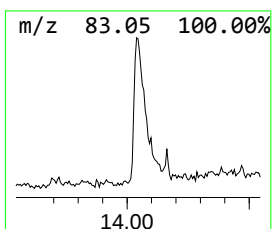
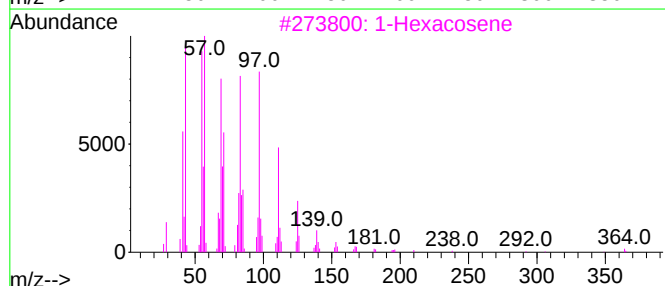
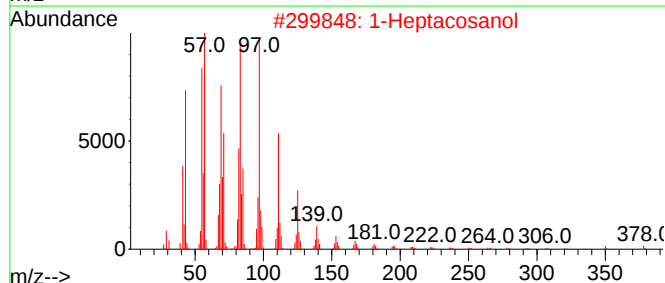
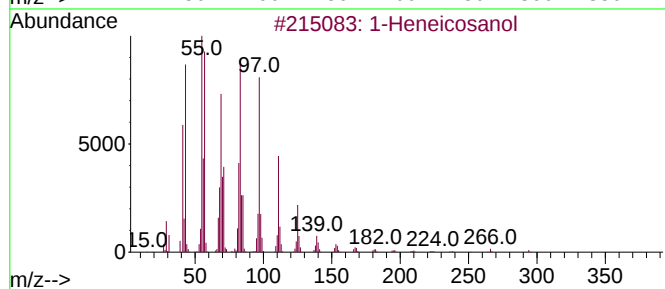
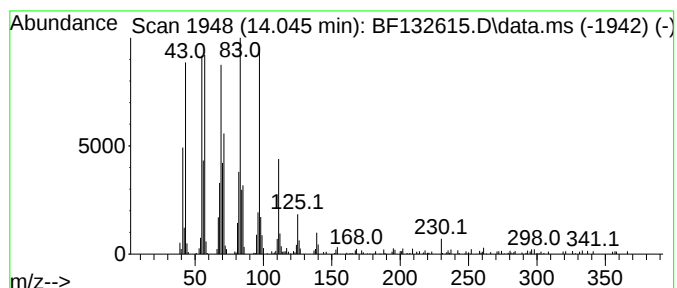
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF022223.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 1-Heneicosanol Concentration Rank 2

| R.T.      | EstConc         | Area   | Relative to ISTD | R.T.        |      |
|-----------|-----------------|--------|------------------|-------------|------|
| 14.045    | 10.18 ng        | 551239 | Chrysene-d12     | 14.204      |      |
| Hit# of 5 | Tentative ID    | MW     | MolForm          | CAS#        | Qual |
| 1         | 1-Heneicosanol  | 312    | C21H44O          | 015594-90-8 | 94   |
| 2         | 1-Heptacosanol  | 396    | C27H56O          | 002004-39-9 | 94   |
| 3         | 1-Hexacosene    | 364    | C26H52           | 018835-33-1 | 93   |
| 4         | Behenic alcohol | 326    | C22H46O          | 000661-19-8 | 92   |
| 5         | 1-Tetracosene   | 336    | C24H48           | 010192-32-2 | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF030223\  
Data File : BF132615.D  
Acq On : 02 Mar 2023 19:14  
Operator : CG\JU  
Sample : 01749-07  
Misc :  
ALS Vial : 12 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
CF-9

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF022223.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| 2-Pentanone, 4-... | 5.240  | 41.2    | ng    | 2485740  | 1                     | 6.998  | 1207610 | 20.0 |
| Cyclohexane, 1-... | 6.698  | 3.2     | ng    | 190843   | 1                     | 6.998  | 1207610 | 20.0 |
| p-Cymene           | 7.069  | 2.4     | ng    | 143336   | 1                     | 6.998  | 1207610 | 20.0 |
| Cyclohexene, 4-... | 7.110  | 2.7     | ng    | 162731   | 1                     | 6.998  | 1207610 | 20.0 |
| n-Hexadecanoic ... | 12.057 | 6.2     | ng    | 407528   | 4                     | 11.545 | 1316380 | 20.0 |
| 1-Heneicosanol     | 14.045 | 10.2    | ng    | 551239   | 5                     | 14.204 | 1083480 | 20.0 |